PB86-112406

SESOIL: A Seasonal Soil Compartment Model

Little (Arthur D.), Inc., Cambridge, MA

Prepared for

Environmental Protection Agency, Washington, DC

May 84

U.S. Department of Commerce
National Technical Information Service
NTIS

PB86-112406

"SESOIL"

A *SE*ASONAL *SOIL* COMPARTMENT MODEL

by

Marcos Bonazountas, and
Janet M. Wagner

Associated with:
Arthur D. Little, Inc. (ADL)
Acorn Park
Cambridge, Massachusetts 02140 USA
617/864-5770 x5871

and

DIS/ADLPIPE, Inc.
55 Wheeler Street
Cambridge, Massachusetts 02138 USA
617/492-1991 x5820

Designed for

Project Officer: Michael A. Callahan
Task Manager: I. Annett Nold
Section Chief: William P. Wood

EPA Contract No. 68-01-6271

United States Environmental Protection Agency
Office of Toxic Substances
Washington, DC 20460
202/382-3926

May 1984

C-85875

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

50272-101

REPORT DOCUMENTATION PAGE

1. REPORT NO. EPA/SW/DF-86/005a
2.
3. Recipient's Accession No. PB86-112406

4. Title and Subtitle

"SESOIL": A SEASONAL SOIL COMPARTMENT MODEL

5. Report Date May 1984
6.

7. Author(s) Arthur D. Little, Inc.

8. Performing Organization Rept. No.

9. Performing Organization Name and Address

U.S. EPA
Office of Toxic Substances TS-798
401 M St. SW
Washington, DC 20460

10. Project/Task/Work Unit No.

11. Contract(C) or Grant(G) No.
(C) 68-01-6271
(G)

12. Sponsoring Organization Name and Address

13. Type of Report & Period Covered Users Guide

14.

15. Supplementary Notes

for magnetic tape see PB36-112398

16. Abstract (Limit: 200 words)

SESOIL is a user-friendly mathematical soil compartment model designed for long-term environmental hydrologic, sediment and pollutant fate simulations.

17. Document Analysis a. Descriptors

Soil flow modeling
Chemical Fate
Transport and transformation

b. Identifiers/Open-Ended Terms

c. COSATI Field/Group

18. Availability Statement

19. Security Class (This Report)

20. Security Class (This Page)

21. No. of Pages 148

22. Price $16.95

(See ANSI-Z39.18)

See Instructions on Reverse

OPTIONAL FORM 272 (4-77)
(Formerly NTIS-35)
Department of Commerce

ABSTRACT

Bonazountas, M. and J. Wagner (1984). SESOIL: A Seasonal Soil Compartment Model. Designed for the U.S. Environmental Protection Agency, Office of Toxic Substances, Washington, D.C. EPA Contract No. 68-01-6271. Arthur D. Little, Inc., Cambridge, Massachusetts, 02140 USA, Telephone No. 864-5770.

SESOIL is a user-friendly mathematical soil compartment model designed for long-term environmental hydrologic, sediment, and pollutant fate simulations. It can describe: water transport (quality and quantity); sediment transport (quality and quantity); pollutant transport and transformation; soil quality; pollutant migration to groundwater; and other processes. Simulations are performed for a user specified soil column extending between the ground surface and the lower part of the unsaturated soil zone of a region. The simulations are based upon a three-cycle rationale, each cycle being associated with a number of processes. The three cycles are the: (1) hydrologic cycle which takes account of rainfall, soil moisture, infiltration, exfiltration, surface runoff, evapotranspiration, groundwater runoff, (2) sediment cycle which takes account of sediment washload (from storms) and sediment resuspension (due to wind), and (3) pollutant fate cycle which takes account of advection, diffusion/volatilization, adsorption and desorption, chemical degradation or decay, biological transformation, hydrolysis, photolysis (not operational), oxidation (not operational), complexation of metals by organic ligands, cation exchange, fixation (not operational), nutrient cycles (not operational) and other processes. Model development has been sponsored by the U.S. Environmental Protection Agency and validation studies have been performed for the hydrologic part of the model (in estimating basin water balances), and for the unsaturated soil zone part of the model (pollutant transport model at waste land treatment disposal sites). The model has been also applied to estimating volatilization of solvents from leaking buried barrels, and to conducting exposure assessment studies. The entire model development has not yet been fully accomplished; however, most model features are operational.

Key Words:

SESOIL, mathematical modeling, pollution, washload, sedimentation, soil quality, groundwater, pathways, land treatment waste disposal, multi-media modeling.

TABLE OF CONTENTS

Page

Abstract ii
Acknowledgements v
SESOIL Model Summary vii

1.0 INTRODUCTION 1-1
2.0 THE SESOIL MODEL 2-1
3.0 USER'S MANUAL 3-1

APPENDICES

HY Hydrologic Cycle HY-1
SW Soil Washload SW-1
SR Soil Resuspension SR-1

VO Diffusion and Volatilization VO-1
AD Adsorption and Desorption AD-1
DE Degradation and Decay DE-1
HD Hydrolysis of Organic Compounds HD-1
CE Cation Exchange CE-1
CM Complexation of Metals CM-1
PH Photolysis (not in this documentation) PH-1
FX Fixation (not in this documentation) FX-1
BI Biologic Uptake (not in this documentation) BI-1
PU Plant Uptake (not in this documentation) PU-1
NU Nutrients Cycle (preliminary study) NU-1
RN Radionuclide Activity (not in this documentation) RN-1
PT Pollutant Fate Cycle PT-1

ID Input Data Compilation ID-1
DF Data Files and Arrays DF-1
FC FORTRAN Code FC-1
AP Applications AP-1
RE References RE-1
MI Miscellaneous MI-1

DISCLAIMER

This document is a working draft which is being circulated for technical review and testing. The contents should not be construed to represent the views and policies of the U.S. Environmental Protection Agency, nor does mention of trade names or commercial products constitute recommendations concerning use.

ACKNOWLEDGEMENTS

This report has been submitted by Arthur D. Little, Inc., in partial fulfillment of the requirements of EPA Contract No. 68-01-6271. The study was performed for the U.S. Environmental Protection Agency, Office of Toxic Substances, Washington, D.C. The authors would like to extend their gratitude to all who have assisted them on this and the previous SESOIL contracts.

To the project officer on this version Mr. *Michael A. Callahan*, Chief of the Exposure Assessment Branch of the Exposure Evaluation Division of the Office of Toxic Substances, the authors give their gratitude, for his support and guidance. To the task manager Dr. *I. Annette Nold* in the Modeling Section of the Design and Development Branch of the same office, the authors extend their thanks for her efforts on this and past SESOIL tasks. Dr. Nold has been patient with the inevitable developmental problems, has contributed to the improvements over the life thus far of the model, and is always ready to compile scientific and other information for us.

Dr. *William Wood*, Chief of Modeling Section in Exposure Evaluation Division of the office of Toxic Substances, and Mrs. *Joan Lefler*, Exposure Integration in the same EPA Division supervised in 1979 the first EPA contract which lead to the conceptualization of SESOIL (Aravamudan et al 1981). The authors appreciate both the scientific advice and the support received until 1984 for the SESOIL concept.

The authors express their graditude to Professor *Peter S. Eagleson*, Massachusetts Institute of Technology, Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, who has contributed in many ways to the SESOIL Development, has voluntarily reviewed and has made suggestions for the application of his annual water balance theory (Eagleson 1978) in respect to the long-term (averaged) estimates of pollutant concentrations in the unsaturated soil zone of SESOIL. See Appendix HY of this documentation.

The authors express also their gratitudes to both, Professor Dr. *George R. Foster*, Purdue University, and Dr. *Walter G. Knisel*, Department of Agriculture, for the assistance received while working out for SESOIL the adaptation of their new (August 16, 1982) erosion model EROS-II, an earlier version of which has been presented in the CREAMS model (Knisel, editor 1980). See Appendix SW of the SESOIL documentation.

Following its conceptualization in 1979, a model improvement and an application were sponsored in 1980 by the EPA, Monitoring and Data Support Division (MDSD), Office of Water Regulations and Standards. Mr. *Michael Slimak*, at the head of the MDSM, has been the Project Officer, and Mr. *John Segna* supervised that task. The authors appreciate the overall advice of John Segna and the support received from this EPA office.

Special thanks are extended to the *Arthur D. Little, Inc. staff* members, who have contributed extensively to this original scientific effort. They are: Diane Gilbert, Warren Lyman, Liz Marchany, Sigfried Mathias, Marise Mikulis, Linda Nappi, Linda Nazaretian, Joo Hooi Ong, Irene Richabaugh, Kate Scow, and Hans Sachdeva.

The authors would like to thank *I.W. Dingwell*, president of DIS/ADLPIPE, Inc. for his patience and support during this project, *Virginia Sullivan* for assistance with the accounting, and *Betty Kenney* and *Carole Doyle* for their assistance with the documentation.

Finally, the authors like to thank Ms. *Gayaneh Contos* at Versar, Inc., and Dr. *George Harris*, at Arthur D. Little, Inc., who have managed this contract with the EPA, Dr. *Alfred Wechsler*, Dr. *Alan Eschenroeder*, Dr. *Philip Levins*, Dr. *Frank Feeley*, and Dr. *Joan Berkowitz*, who have supported us in many different ways.

SESOIL MODEL SUMMARY

GENERAL INFORMATION

SESOIL is a user-friendly mathematical model for long-term environmental pollutant fate simulations that is designed to describe:

- water transport (quality/quantity),
- sediment transport (quality/quantity),
- pollutant fate (transport/transformation),
- pollutant migration to groundwater,
- soil quality, and
- other processes.

within a user specified soil column (consisting of many compartments), which extends between the ground surface and the lower part of the saturated soil zone of a region. *(Figure 1)*.

SESOIL is designated as "seasonal" because it estimates the pollutant distribution in the soil column and on the watershed after a season (e.g., year, month) "directly" by employing a statistical water balance analysis and a washload routine statistically driven in a season. Thus, SESOIL does not estimate the pollutant distribution by summing up estimates in the soil column after each major storm event as do existing models described in the literature. In that respect the model saves both user professional time to input data and computer time.

SESOIL has been designed to become, in the long run: (1) an unsaturated soil zone model; (2) a watershed model; and (3) a groundwater model. However, the current model version (1984) can not account for the groundwater aspects of SESOIL, which are part of the long-range point or nonpoint pollution from major land use categories, and soil-column pollution originating on the watershed, in the soil column and in groundwater (future development).

SESOIL is designed as: (1) a self-standing soil compartment model, and (2) a compartment model to be interfaced with other atmospheric and water body models towards the formation of a mathematical environmental continuum (multi-media environmental modeling, e.g., Hetrick 1984). The current version can be easily interfaced with a groundwater model toward the formulation of an unsaturated/saturated soil compartment model, in order, for example, to trace pollutants from the disposal site to-the-well.

SESOIL simulations do not require the extensive and time consuming calibration procedures of other models, although the model may be easily calibrated to agree with field records. The model employs theoretically derived equations driven by climatic, soil property, geometric and chemical compound property data. In addition, simulations are performed for the entire compartment (i.e., watershed, unsaturated soil zones) in one effort, in order to circumvent the known calibration difficulties of simulation models. As such, SESOIL may be employed as a pre-calibration model for other simulation models — especially hydrologic/water balance models.

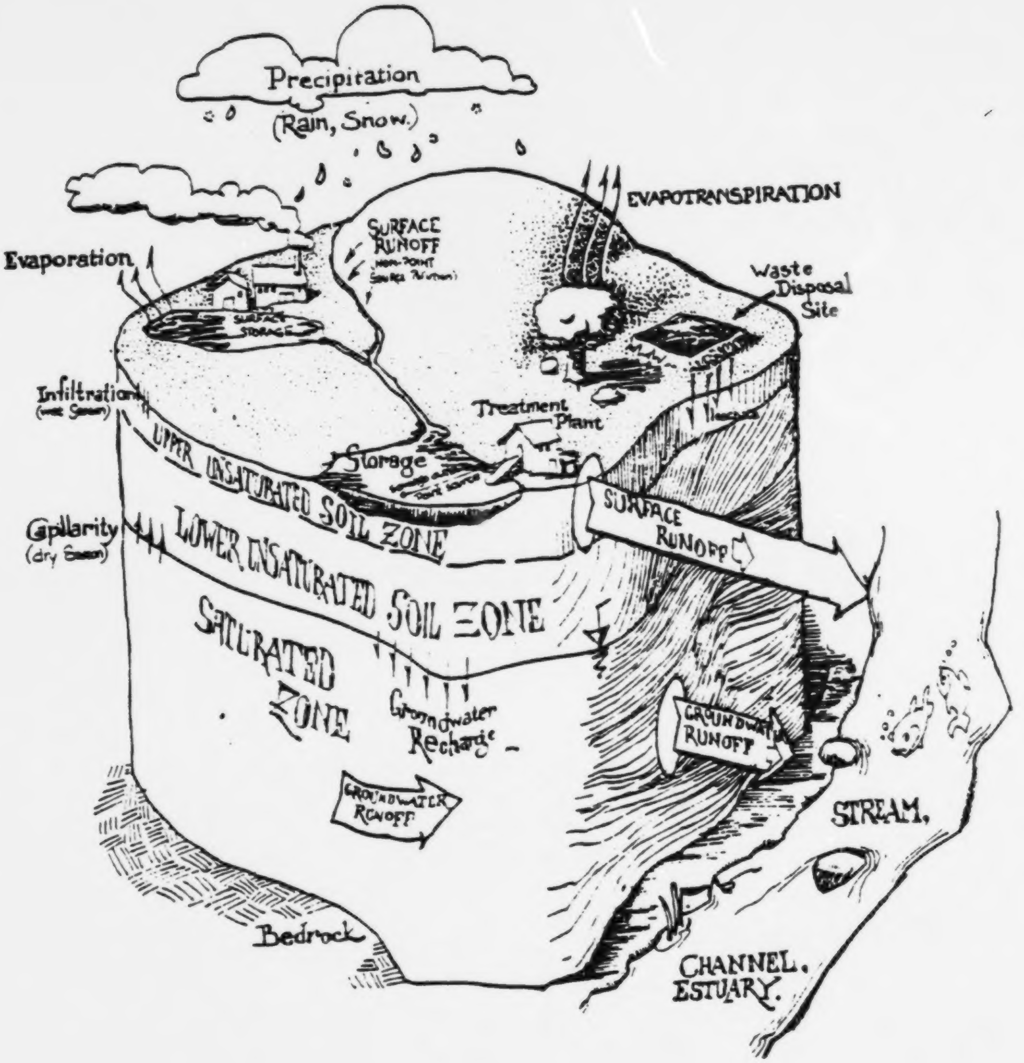

Precipitation
(Rain, Snow.)
EVAPOTRANSPIRATION
Evaporation
SURFACE RUNOFF
Waste Disposal Site
SURFACE STORAGE
Infiltration
(wet Season)
Treatment Plant
Storage
UPPER UNSATURATED SOIL ZONE
Capillarity
(dry Season)
LOWER UNSATURATED SOIL ZONE
SURFACE RUNOFF
SATURATED ZONE
Groundwater Recharge
GROUNDWATER RUNOFF
GROUNDWATER RUNOFF
STREAM.
Bedrock
CHANNEL.
ESTUARY.

FIGURE 1 SCHEMATIC PRESENTATION OF THE SESOIL ENVIRONMENT

There exist no artificially imposed limitations in: (1) timing and sizing the soil compartment (cell), and (2) the shape of the compartment per se. If the soil column is chosen small enough (i.e., finite approach), SESOIL encompasses the concept of the numerical models (e.g., finite difference or element models); if the soil column is chosen large enough (e.g., a river basin), SESOIL becomes a one-compartment watershed model, although no attention is given to the spatial distribution of the rainfall (Eagleson 1984). The unsaturated soil zone of the model can be discretized to account for more than one soil layer in order to best meet simulation needs. However, user judgment is needed for the timing and spacing to be correct.

SESOIL is designed to provide great flexibility to the user who can execute various "options" of model operation, the criterion for an option selection being data availability and study objectives. The major advantage of SESOIL is that it can be executed with easily obtainable input data because this information can be compiled from existing data bases (e.g., NOAA) and known references for the pollutant and soil properties (e.g., Lyman et al 1982). A data management structure accompanies SESOIL. If the model is not linked to existing data bases, then the number of input data can be less than 50 — as contrasted to the other numerical models which may require more than 500 — because: (a) the model employs theoretically derived equations which do not require calibration via calibration coefficients, and (b) the statistical simulation does not take place after each major storm event.

Potential applications of SESOIL include long-term leaching studies from waste disposal sites, acid rain, pesticide and sediment transport on watersheds, contaminant exposure assessments, pre-calibration runs for other simulation models, hydrologic cycles and water balances of soil compartments, overall chemical fate assessments, exposure, risk and other studies.

This model version has been developed on behalf of the U.S. Environmental Protection Agency, Office of Toxic Substances, Washington, D.C. A model application at industrial land treatment sites has been sponsored for a sightly different model version by the Monitoring and Support Data Division, EPA, Washington, D.C.

SIMULATION CYCLES

The SESOIL simulations are structured around three cycles, each cycle being associated with a number of processes. They are the:

- Hydrologic cycle which takes account of: rainfall, infiltration, soil moisture, surface runoff, exfiltration, evapotranspiration, groundwater runoff, capillary rise, snow pack/melt (not operational in this version) and interception (not operational).

- Sediment cycle which takes account of: sediment resuspension (due to wind) and sediment washload (due to rain storms).

- Pollutant fate cycle which takes account of: advection, diffusion, volatilization, adsorption and desorption, chemical degradation or decay, biological transformation, hydrolysis, cation exchange, complexation chemistry (metals by organic ligands), and other processes.

The hydrologic cycle controls the sediment cycle, whereas both previous cycles control the pollutant fate cycle. Cycles, processes, mathematical modeling, application and validation issues are summarized in the following paragraphs.

The hydrologic cycle is based on a statistical dynamic formulation of vertical water budget at a land-atmosphere interface (Eagleson 1978), adapted to account for monthly simulations and for moisture variations in the soil zone. Uncertainty of the hydrologic cycle simulation is expressed via probability density functions of the independent climatic variables and yields derived probability distributions of the dependent water balance elements: surface runoff, evapotranspiration, and groundwater runoff. Some details of the hydrologic analysis are (Eagleson 1978):

Seasonal point precipitation is represented by Poisson arrivals of rectangular gamma distributed intensity pulses that have random depth and duration. Infiltration and exfiltration are described by the Philip equation (Philip 1969), which assumes the medium to be effectively semi-infinite, and the internal soil moisture at the beginning of each storm and inter-storm period to be uniform at its long-term space-time average. Gravitation and percolation to groundwater is assumed to be steady throughout the time step of a simulation and at a rate determined by the long-term space-time average seasonal soil moisture. Capillary rise from the water table is assumed to be steady throughout the season and to take place to a dry surface. Soil properties, soil moisture, climate and functional relationships derived by Brooks and Corey (1966) describe the wetting drying soil intrinsic permeability temporal variation.

Seasonal bare soil evaporation and vegetal transpiration are calculated for the interstorm periods as functions of properties of the climate, the storm sequence, the surface, the soil and the average rate of a derived potential evapotranspiration. The work of Penman (1963), Van den Honert (1948), Cowan (1965) is employed (Eagleson 1978). The distribution of surface runoff volume is derived from the distribution of rainstorm intensity and duration and the use of the previously discussed infiltration equation. Specific subroutines of the model have been validated in the literature. The annual dynamic water balance of the model has been validated by Eagleson (Eagleson 1978). The monthly dynamic water balance of the model has been applied and validated by various scientists (Watson and Brown 1984). Validation of the routine was undertaken in connection with hydrologic simulation or with pollutant migration in the unsaturated soil zone (Bonazountas and Wagner 1982).

Sediment cycle can potentially account for both, sediment (washload) due to precipitation and sediment (dust) resuspension due to wind. The theoretical monthly washload routine can account for: (a) various sizes and shapes of washsheds (e.g., overland flow, channel flow, impoundment, pond); (b) attachment of soil particles, transport and deposition of soil particles, rill and inter-rill erosion on the watershed; (c) sediment characteristics and other fundamental relationships of precipitation energy and erosion sediment transport. The sediment washload model is based on the fundamental theoretical models of Yalin (1963), Foster et al (1980), and

Cooley (1980), as developed by Foster et al (1982) for the CREAMS model (Knisel 1980), however, adopted to the statistical needs of SESOIL for monthly yields and maximum yields of individual storms within a month.

The dust resuspension routine estimates the losses from the surface of the SESOIL soil column of any pollutants associated with surface particles. The losses due to physical removal of the particles that have an associated pollutant load are calculated as a function of particle characteristics (chemical composition, diameter, etc.) and weather conditions. Variables such as soil moisture and wind speed are utilized; however, this routine has not been coded and validated yet with SESOIL's hydrologic cycle.

The pollutant fate cycle accounts for more than 12 chemical processes. There exists no single equation that can optimally describe each of the pollutant processes under all conditions, so some alternative simulation options are possible; for example, adsorption is modeled as sorption to soil particles, partitioning to soil organic carbon, or as an ion exchange process; by varying the input parameters. Another example is volatilization from soil to air that can be modeled with more than one user specified equation (theoretical, experimental).

The pollutant fate cycle is simulated in more than one soil subcompartments, each one consisting of three phases: soil-air, soil-moisture and soil-solids. The pollutant fate cycle routine has been re-derived from a pollutant mass balance equation that can be expanded or modified easily in order to account for additional processes and model improvements.

MODEL APPLICATIONS

A pollutant transport application/validation study was undertaken to assess the long-term predictive pollutant pathway capabilities of SESOIL using field monitoring data and supporting background information already collected as part of another study (monitoring program). The model has been employed as (1) an upper unsaturated soil zone model at two industrial land treatment waste sites, and (2) as an exposure assessment model for hypothetical environmental soil compartments. The behavior of two organic pollutants (naphthalene, anthracene) and four inorganic pollutants (copper, chromium, nickel, sodium) at two sites was simulated and analyzed. Predicted concentrations and laboratory measured concentrations agreed within expected limits. Calibrated and noncalibrated model runs have been compared (Bonazountas et al 1982).

SESOIL has also been employed as a mathematical tool for exposure assessment studies for predicting the behavior of pollutants (e.g. volatile compounds) in soil compartments, and it proved to be an interesting application for screening, analyzing and prioritizing pollutant behaviors in soil systems (Wagner and Bonazountas 1983).

In order to evaluate existing geohydrochemical models, Battelle Pacific Northwest Laboratories have established model performance criteria and have evaluated about 100 available model codes applicable to leachate migration from waste disposal sites. Among the 21 codes selected has been the SESOIL code also (Murarka 1984).

SESOIL testing is conducted by Watson and Brown (1984). Testing includes comparative analyses of SESOIL model predictions with both field data and predictions of other models describing the movement of toxic chemicals on the watershed and the soil zone of a region. The SESOIL model and four other models are applied at four agricultural sites (Florida, Long Island, Georgia, Iowa).

SESOIL has been also applied, tested (or recommended for testing), by the Oak Ridge National Laboratory for river basin simulations; Battelle Pacific Laboratory for hydrologic cycles at waste sites; the EPA-EMSL Laboratory, Las Vegas, for laboratory soil column tests of pollutant leachates; the EPA — Office of Solid Waste; the EPA — Clearinghouse, the Harvard University School of Public Health; the EPA Corvallis Research Laboratory, the ICF Corporation on behalf of the EPA/OTS; the GCA Corporation on behalf of the EPA; the Midwest Research Institute, Kansas City for Health Risk Assessment Methodologies; the National Technical University of Athens, Greece, for hydrologic balances; and other institutions. Finally, the General Software Corporation in Maryland has developed for the EPA/OTS an interactive supporting system for SESOIL and the EPA/OTS Graphical Exposure Modeling System (GEMS) (GSC 1983).

REFERENCES

Aravamudan, K., M. Bonazountas, A. Eschenroeder, D. Gilbert, L. Neklen, K. Scow, R. Thomas, W. Tucker, G. Unger (1981). An Environmental Partitioning Model for Risk Assessments of Chemicals. EPA/OTS Contract No. G8-01-3857. Draft Report. Arthur D. Little, Inc., Cambridge, MA 02140.

Bonazountas, M., J. Wagner, and B. Goodwin (1982). Evaluation of Seasonal Soil/Groundwater Pollutant Pathways. Arthur D. Little, Inc., Final Report, prepared for U.S. EPA, Monitoring and Data Support Division. EPA Contract No. 68-01-5949/9.

Bonazountas, M., J. Wagner, and B. Goodwin (1981). Seasonal Cycles of Pollutants Originating from Land Treatment Practices. Proceedings Environmetrics '81 Conference, SIAM/SIMS, Virginia.

Brooks, R.H. and A.T. Corey (1966). Properties of Porous Media Affecting Fluid Flow. Proc. ASCE Journal of the Irrigation and Drainage Division, No. IR 2, Paper 4855, pp. 61-68.

Cooley, R.K. (1980). Erosivity "R" for Individual Rain Storms. (In Knisel, p. 386.)

Cowan, J.R. (1965). Transport of Water in the Soil-Plant-Atmosphere System. J. App. Ecology (2):221-239.

Eagleson, P.S. (1984). The Distribution of Catchment Coverage by Stationary Rainstorms. Water Resources Research, Vol. 20(5):581-590.

Eagleson, P.S. (1978). Climate, Soil, and Vegetation (1-7). Water Resources Research, Vol. 14(5):705-706.

Foster, G.R., L.J. Lane, J.D. Nowlin, J.M. Laflen, and R.A. Young (1980). A Model to Estimate Sediment Yield from Field-Sized Areas: Development of Model. Purdue Agricultural Experiment Station. Purdue Journal No. 7781.

GSC — General Software Corporation (1983). User's Guide to SESOIL Execution using the Data Management Supporting System, SESIN and SESOIL. EPA Contact No. 68-01-16618, Draft Report. USEPA, Office of Pesticides and Toxic Substances, Exposure Evaluation Division, Washington, DC 20406.

Hetrick, D.M. (1984). TOX-SCREEN: A Multimedia Screening Level Program for Assessing the Potential Fate of Chemicals Released to the Environment. Prepared for EPA/OTS, Contract No. W-7405-Eng-26, by Oak Ridge National Laboratory, TN 37830, USA.

Knisel, W.G. (1980). CREAMS: A Field Scale Model for Chemicals Runoff and Erosion for Agricultural Management Systems. USDA Conservation Research Report No. 26.

Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt (1982). Handbook of Chemical Property Estimation Methods. McGraw-Hill, Inc., NY, NY. ISBN 0-07-039175-0

Murarka, I. (1984). EPRI Journal. Page 53. Palo Alto, California.

NOAA (National Oceanographic and Atmospheric Administration). Local Climatological data files, Monthly Climatologic data.

Penman, H.L. (1963). Natural Evaporation from Open Water, Bare Soil, and Grass. Proc. Roy. Soc. (London), Ser. A, Vol. 193, 1948, pp. 120-145.

Philip, J.R. (1969). Theory of Infiltration, in Advances in Hydroscience, Vol. 5, edited by V.T. Chow, pp. 215-296. Academic Press, New York.

Van den Honert, T.H. (1948). Water Transport in Plants as a Catenary Process. Discuss. Faraday Soc. 3:146-153. (Cited from Eagleson 1978.)

Wagner, J. and M. Bonazountas (1983). Buried Halogenated Solvent Simulations via SESOIL. Arthur D. Little, Inc., study in progress, performed for U.S. EPA, Office of Toxic Substances. EPA Contract No. 68-01-6271.

Watson, D. and S. Brown (1984). Recommendation Testing Procedures for the SESOIL Model. EPA Contract No. 68-03-3116. Anderson-Nichols & Co., Inc., Palo Alto, California 94303 USA.

Wischmeier, W.H. and D.D. Smith (1978). Predicting Rainfall Erosion Losses. U.S. Department of Agriculture, Agriculture Handbook No. 537.

Yalin, Y.J. (1963). An Expression for Bedcover Transportation. Journal of the Hydraulics Division. Proceedings of the ASCE 89(HY3):221-250.

Page

CHAPTER 3.0 — USER'S MANUAL

3.1 BACKGROUND 3-5

- 3.1.1 General SESOIL Capabilities 3-5
- 3.1.2 Pheonomenology in the Soil Compartment 3-5
- 3.1.3 Mathematical Modeling issues 3-9
- 3.1.4 SESOIL Operations (Options) 3-10
  - 3.1.4.1 General 3-10
  - 3.1.4.2 OPTION 0 3-11
  - 3.1.4.3 OPTION A 3-11
  - 3.1.4.4 OPTION M 3-13
  - 3.1.4.5 Other Options 3-15
- 3.1.5 Canonical/Scenario Chemical Fate Modeling 3-15

3.2 DATA STRUCTURE/MANAGEMENT 3-16

- 3.2.1 General 3-16
- 3.2.2 SESOIL Program and Data Structure 3-16
- 3.2.3 Model Execution Philosophy 3-18
- 3.2.4 Input Data Files 3-18
  - 3.2.4.1 ANNUAL DATA File 3-19
    - 3.2.4.1.1 General 3-19
    - 3.2.4.1.2 ANNUAL Data Input 3-21
  - 3.2.4.2 CLIMAT DATA File 3-24
    - 3.2.4.2.1 General 3-24
    - 3.2.4.2.2 CLIMAT Data Input 3-26
  - 3.2.4.3 SOIL DATA File 3-28
    - 3.2.4.3.1 General 3-28
    - 3.2.4.3.2 Data Input 3-28
  - 3.2.4.4 CHEM DATA File 3-30
    - 3.2.4.4.1 General 3-30
    - 3.2.4.4.2 CHEM Data Input 3-32
  - 3.2.4.5 APPLIC DATA File 3-34
    - 3.2.4.5.1 General 3-34
    - 3.2.4.5.2 APPLIC Data Input 3-34
  - 3.2.4.6 WASH DATA File 3-40
    - 3.2.4.6.1 General 3-40
    - 3.2.4.6.2 Data Input 3-40
  - 3.2.4.7 EXEC DATA File 3-43
- 3.2.5 Summary of Data Input 3-45

Page

3.3 MODEL EXECUTION 3-53

3.3.1 Date Requirements 3-53
3.3.2 Execution Statement 3-53
3.3.3 Examples of Execution 3-53

3.4 MODEL "VALIDATION" 3-55

3.4.1 General 3-55
3.4.2 Model Application 3-55
3.4.3 Model Galibration 3-57
3.4.4 Model Validation 3-61
3.4.5 Model Sensitivity Analysis 3-64
3.4.6 Modeling Precision and Error Analysis 3-64
3.4.7 Model Limitations 3-66
3.4.8 Discussion 3-66

3.5 REFERENCES 3-68

LIST OF TABLES

Table No. Page

3-1 ANNUAL DATA File (Overview)

3-2 CLIMAT DATA File (Overview)

3-3 SOIL DATA File (Overview)

3-4 CHEM DATA File (Overview)

3-5 WASH DATA File (Overview)

3-6 APPLIC DATA File (Overview)

3-7 EXEC DATA File (Overview)

3-8 Soil Quality Modeling; Major Input Parameter Categories

3-9 References of Current Rsearch (1979) in Calibration/ Validation Procedures for Soil/Groundwater Models

LIST OF FIGURES

Figure No. Page

3-1 Principal Environmental Pathways of Toxic Substances

3-2 Physical and ~~Biogeochemical~~ Pollutant Fate Processes Estimated by SESOIL

3-3 Compartment Disaggregation; OPTION O, OPTION A

3-4 Compartment Disaggregation; OPTION M

3-5 Overview of Major Subroutines and Data Files

3-6 ANNUAL DATA File

3-7 CLIMAT DATA File

3-8 SOIL DATA File

3-9 CHEM DATA File

3-10 APPLIC DATA File

3-11 WASH DATA File

3-12 EXEC DATA File

3-13 Schematic of Model Application, Calibration, Validation

3.0 USER'S MANUAL

3.1 BACKGROUND

In this user's manual (Chapter 3.0) it is assumed that the reader (model user) is familiar with the theory, the constraints, and the terminology of the SESOIL model.

3.1.1 General SESOIL Capabilities

This version (1984) of SESOIL can be used as:

(1) a hydrologic cycle model for the watershed and the unsaturated soil zone of the compartment,

(2) as hydrologic and a sedimentation (washload) model for the watershed of the compartment, and

(3) as a hydrologic, a washload and a pollutant (geochemical) cycle model for the unsaturated soil zone of the compartment.

SESOIL is still under development (1984).

The following sections guide a user through details and the input/output data of this model version.

3.1.2 Phenomenology in the Soil Compartment

A soil "compartment" (or cell) is defined as a soil column extending between the ground surface and ~~the bottom of~~ the "upper" saturated soil zone. As such, the soil compartment interacts with the air and the water compartments of an environment as schematically shown in the cover figure of this report and in Figure 2-1. It is evident that underlying the upper saturated soil zone will be impermeable soil layers and other saturated soil zones (or aquifiers); however, these zones are not part of the soil compartment simulated by SESOIL in its present version.

Physical and chemical processes or phenomena of importance to the quality of a soil compartment are the hydrologic (or water balance) cycle, the sediment (or washload) cycle, and the pollutant fate cycle. Terminology and processes important to each cycle are described in both the appendices HY through PT of this documentation, and the ACS publication of Bonazountas (1983).

When released into the environment, pollutants distribute by a numberof fate (transport and transformation) mechanisms. Many pollutants are transported primarily through the hydrologic cycle or the hydrologic mechanisms of watersheds and have a final destination in the water compartment of an environment. For some pollutants such as phosphorus, ammonia and certain more highly adsorbing pesticides, surface runoff, soil wash and dust particles might be the primary carriers. Other pollutants are directly applied to plants and reach the soil through drift, wash-off or when the plant decays. Figure 3-1 is a generalized pathway diagram of toxic substances in the environment showing most pathways from source-to-receiver. The SESOIL model deals with processes interacting and related to the soil compartment of the environment; that is, the "elliptic" subcompartment in Figure 3-1.

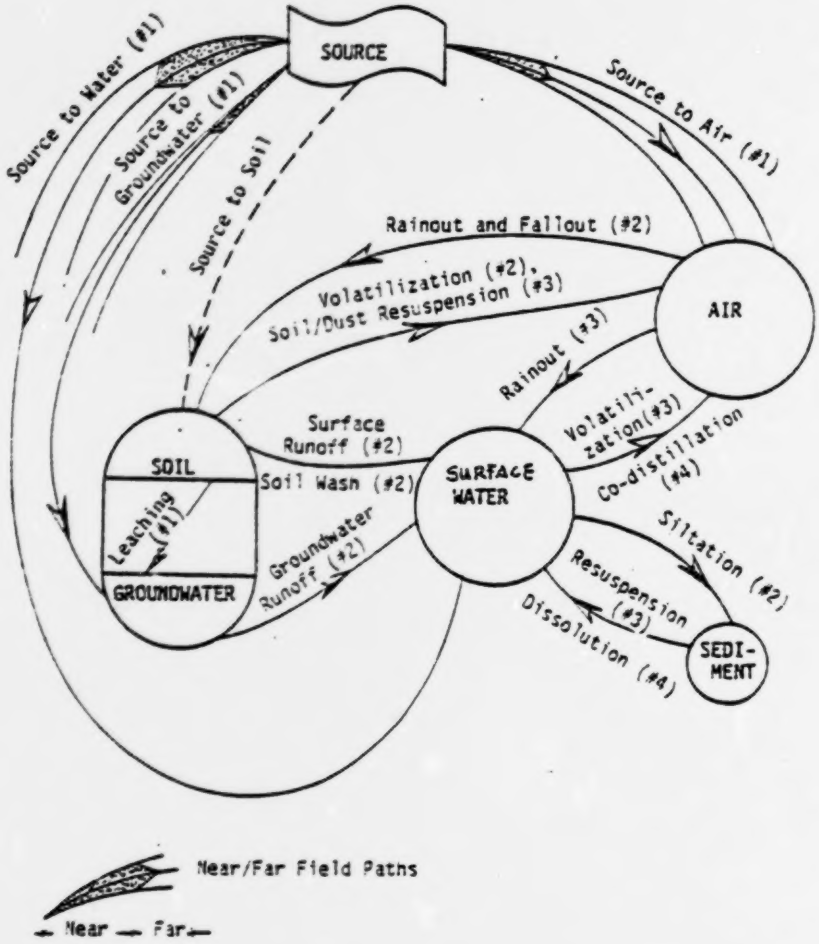
The manner in which pollutants enter the compartmental cycles depends on the characteristics of the pollutant source, such as location, time and physical or chemical form of pollutant. Gaseous, emulsified and dispersed airborne pollutants enter water by precipitation and/or dry fallout. Soluble pollutants and/or pollutants suspended in the water may then enter the soil. Relatively insoluble pollutants discharged to water or soil either are dispersed or are transported by stormwater runoff or are entrained by wind and subsequently redeposited. Pollutants are also adsorbed and desorbed by soil particles and then can be transported by the water cycle in either state (Bonazountas & Fiksel 1982).

A major characteristic of a soil compartment -- as contrasted to a water or an air compartment -- is that the temporal, physical and the chemical behavior of the compartment are governed by both: (1) out-compartmental parameters (forces) such as precipitation, air temperature, solar radiation, and (2) in-compartmental parameters such as soil structure and biogeochemistry parameters. This characteristic is also one of the main reasons why soil compartmental mathematical modeling is more complex than water or air modeling.

When dealing with mathematical modeling of pollutant transport in soil compartments, it is natural to study pollutant migration in the hierarchical order: (1) hydrologic cycle, (2) sediment cycle, which is primarily governed by the first cycle, and (3) pollutant fate cycle, which is primarily governed by the two previous cycles. It has been however, a frequent practice to model pollutant migration based upon soil-moisture migration, so that no soil moisture presence results in no pollutant migration. Although the latter is not the case in SESOIL (eg. see appendix VC), the logical hierarchy: hydrologic cycle, sediment cycle, pollutant cycle has been followed in this modeling effort.

Cycles and processes modeled in SESOIL are shown in Figure 3-2 and are summarized as follows:

(1) Hydrologic cycle which takes account of: rainfall, infiltration, soil moisture, surface runoff, exfiltration, evapotranspiration, soil moisture retention in the root zone, groundwater runnoff, capillary rise, snow pack/melt


SOURCE
Source to Water (#1)
Source to Groundwater (#1)
Source to Soil
Source to Air (#1)
Rainout and Fallout (#2)
Volatilization (#2),
Soil/Dust Resuspension (#3)
AIR
Rainout (#3)
SOIL
Leaching (#1)
GROUNDWATER
Surface Runoff (#2)
Soil Wash (#2)
Groundwater Runoff (#2)
SURFACE WATER
Volatilization(#3)
Co-distillation (#4)
Siltation (#2)
Resuspension (#3)
Dissolution (#4)
SEDIMENT
Near/Far Field Paths
Near
Far

#1. Direct discharge pathways.

#2-4 Intermedia discharge pathways (primary, secondary, potential).

Degradation of substances can take place in any compartment.

Out-of and into basin transfers are not shown.

Source: Bonazountas & Fiksel (1981)

FIGURE 3-1 Principal Environmental Pathways of Toxic Substances

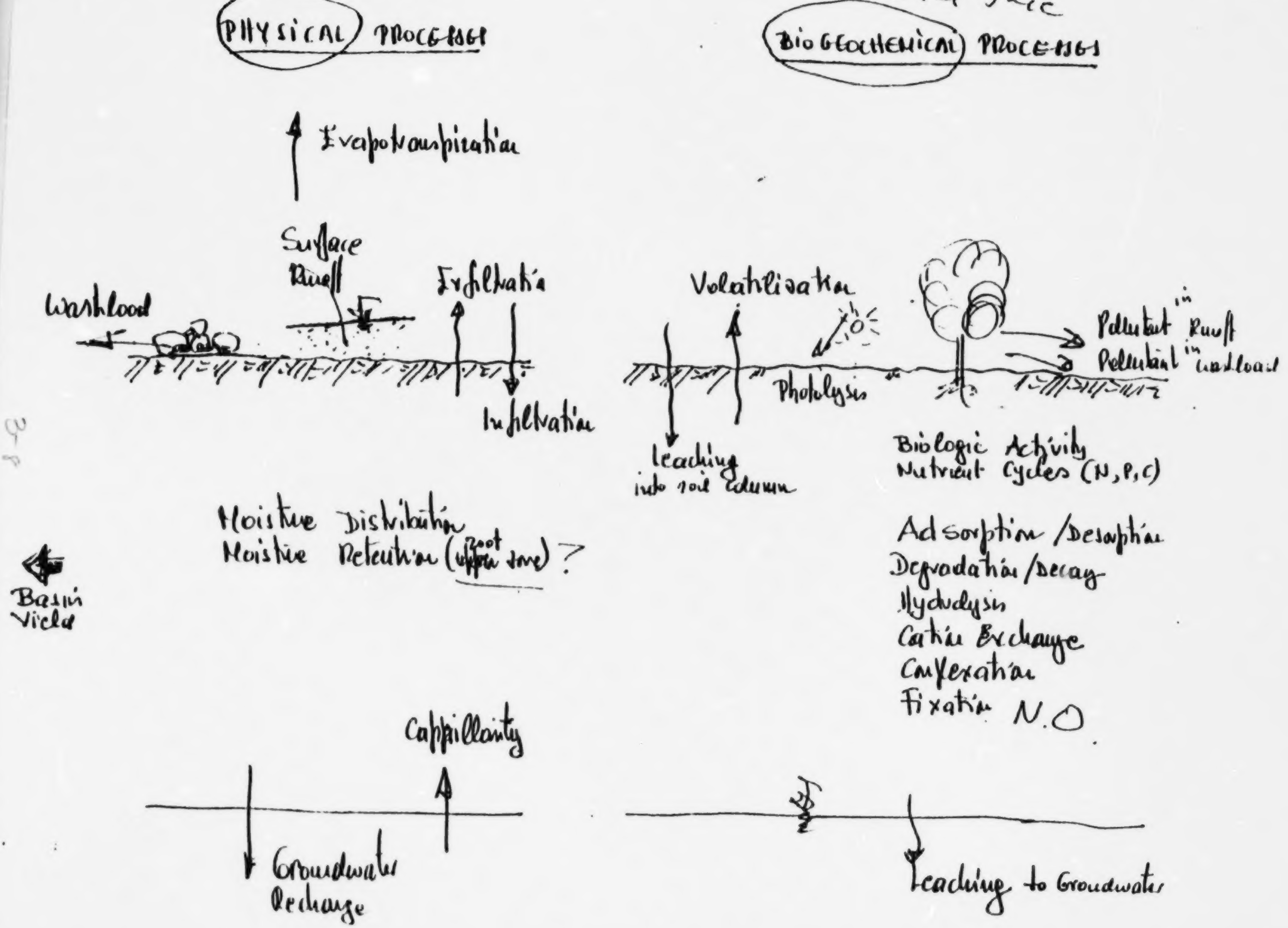

PHYSICAL PROCESSES
BIOGEOCHEMICAL PROCESSES
Evapotranspiration
Surface Runoff
Washload
Exfiltration
Infiltration
Volatilization
Photolysis
Leaching into soil column
Pollutant in Runoff
Pollutant in washload
Biologic Activity
Nutrient Cycles (N, P, C)
Moisture Distribution
Moisture Retention (root upper zone)?
Adsorption /Desorption
Degradation /Decay
Hydrolysis
Cation Exchange
Complexation
Fixation N.O
Basin Yield
Cappillarity
Groundwater Recharge
Leaching to Groundwater

FIGURE 3-2 Physical and Biogeochemical Processes Estimated by SESOIL

Formalize all [illegible]

(not operational in this version) and interception (not operational).

(2) Sediment cycle which takes account of: sediment washload due to rain storms, and sediment resuspension due to wind (not operational).

(3) Pollutant fate cycle which can take account of: advection, diffusion (air phase), volatilization, adsorption and desorption, chemical degradation or decay, biological transformation biological uptake (not operational), hydrolysis, photolysis (not operational), oxidation, photolysis (not operational), oxidation (not operational), cation exchange, complexation (metals by organics), and nutrient cycles (not operational).

3.1.3 Mathematical Modeling Issues

Environmental mathematical models can be classified in general into: deterministic models which describe the system in cause/effect relationships, and stochastic models which incorporate the concept of risk, probability or other measures of uncertainty. Deterministic and stochastic models may be developed from: observation, semi-empirical approaches, and theoretical approaches. In developing a model, scientists attempt to reach an optimal compromise among the above approaches given the level of detail justified by both the data availability and model objectives (Bonazountas 1983).

Deterministic models can be classified into simulation models which employ a well accepted empirical equation that is forced via calibration coefficients to describe a system, and analytic models in which the derived equation describes the physics/chemistry of a system. Both the simulation and the analytic models can employ numerical solution procedures for their equations. Although the above terminology is not standard in the literature, it has been used here as a means of outlining some of the concepts of modeling relevant to SESOIL.

This SESOIL version employs the stochastic approach for both the hydrologic and the washload cycles, and the deterministic approach for the other physical or chemical processes. Parameters of simulation of empirical models are determined by calibrating the model output against large masses of observational data. This procedure involves curve-fitting and least-squares analyses, and requires extensive field data information. In order to by-pass many calibration difficulties, SESOIL employs primarily theoretically developed stochastic or deterministic routines. The model input variables describe physical or chemical parameters and can be determined or obtained independently either from laboratory analyses, or from field investigation, handbooks and data bases.

The choice of theoretical stochastic or analytic deterministic models does not imply — of course — that these models are always superior to empirical or simulation models. The desire for an alternate approach was of importance, therefore a "modular" structure has been employed for SESOIL, so that a substitution of a particular equation, theory, or subroutine (modules) can be undertaken in a straightforward manner. To achieve effectiveness in the modular approach a new, efficient and chemistry-strong concept has been employed for the pollutant fate transport cycle (appendix PT) of SESOIL.

3.1.4 SESOIL Operations (Options)

3.1.4.1 General

Discussions in the following sections are oriented towards the conceptual approaches employed in this methodology and are not intended to fully describe the fundamentals of all the cycles -- hydrologic, washload, and pollutant fate geochemical. For detailed information the reader is referred to the individual appendices.

SESOIL is designed to encompass a variety of features. It can be used, for example, as a watershed model for runoff, sediment and pollutants; and as an unsaturated soil zone hydrogeologic or pollutant fate model. The model can be used for annual or monthly simulations; and for two, three or four soil layers (this model version).

In order to: (1) take advantage of the flexible temporel and spatial resolution design of SESOIL, (2) reduce the input data requirements for certain model uses, and (3) make model user friendly, three model "operation options" are offeredin the form of "integrated packages." The three options are:

OPTION 0	(Option "zero"),
OPTION A	(Option "Annual"), and
OPTION M	(Option "Monthly")

In summary:

> OPTION 0 simulates (models) only pollutant fate cycles with user specified hydrocycle (water balance) and washload cycle components. SESOIL is used as a compartmental soil cell routine for 2 soil cells (layers), for a one year (annual time step) simulation.
>
> OPTION A simulates all cycles (hydro, washload, geochemistry) for 2 soil layers on an annual basis.
>
> OPTION M simulates all cycles for 2, 3, or 4 soil layers on a monthly basis.

Details on the three options (0,A,M) are provided in the following section. In general: OPTION 0 can be operated with a minimum of 46 input parameters (numbers) per simulation; OPTION A with a minimum of 49 input parameters per year; and OPTION M with a minimum of 75 input parameters per month. This information provides a feeling for the nature of complexity of each option.

3.1.4.2 OPTION 0 -- Annual Simulation; User Supplied Water Balance

OPTION 0 is the simplest operational version of the model and does not require knowledge of the climatic and storm parameters of the compartment (area modeled). SESOIL is employed as an unsaturated soil zone model interacting hydrologically (for mass balance purposes) with both the watershed and the groundwater table.

The simulation is performed annually and for only one year. The unsaturated soil zone compartment consists of only two distinct layers, as shown in Figure 3-3, namely the upper unsaturated soil zone (or watershed zone), and the lower unsaturated soil zone. The saturated soil (groundwater) zone is not part of this model option.

The user has to input: (1) the annual averaged values of rainfall depth, soil moisture (unsaturated soil zones), infiltration, groundwater recharge depths and washload mass; (2) the total annual pollutant load (pollutant mass) to the compartment; (3) chemical (compound) related parameters; and (4) soil related paramaters.

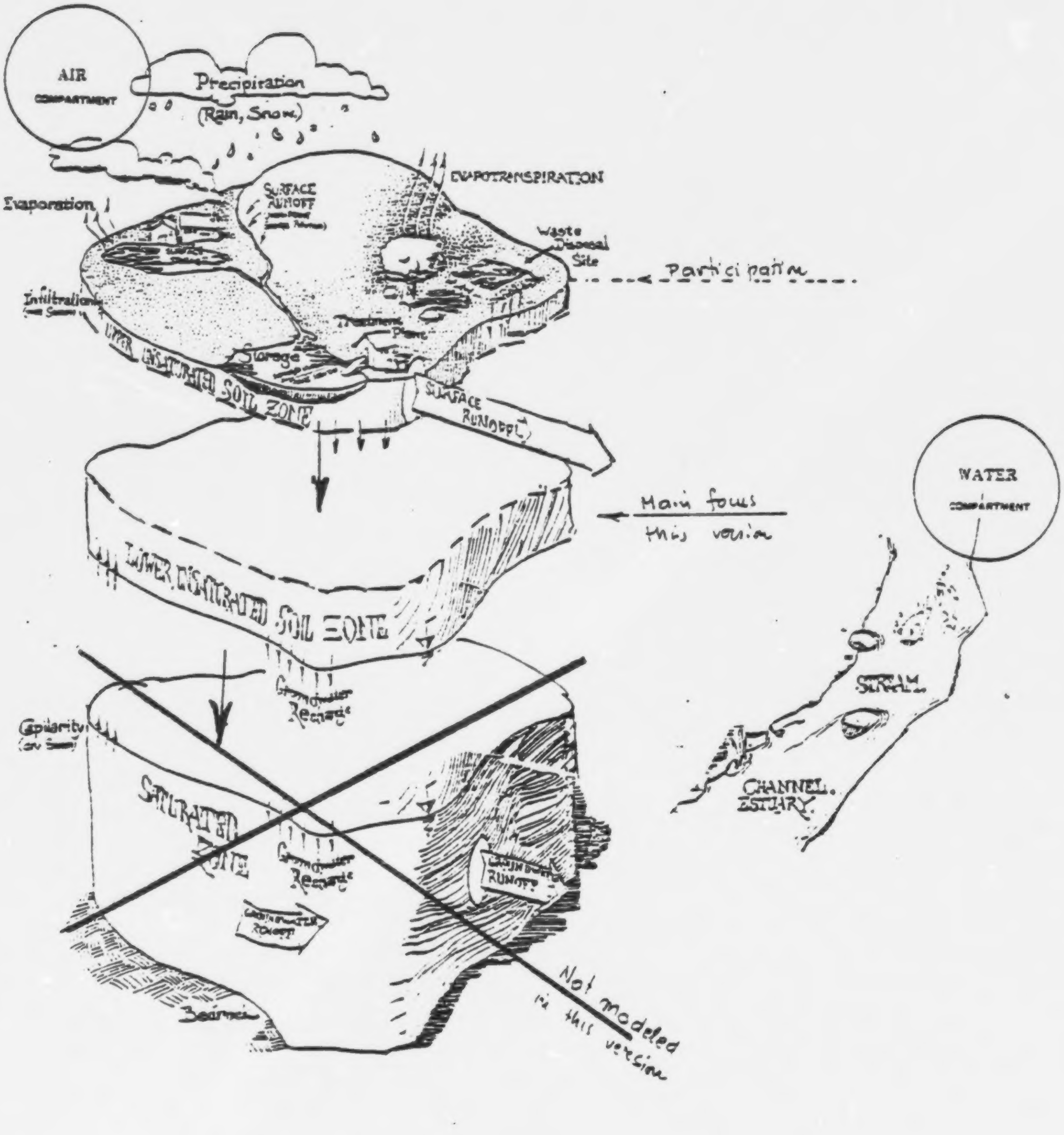
The output from the model is: (1) the pollutant distribution (i.e. concentrations, mass distribution) in the compartment; and (2) the annual pollutant contribution (transport) to other environmental compartments by means of surface runoff, volatilization, leaching to groundwater, and washload.

Additional information for use of this option is provided in section PT-3.2 (Appendix PT). Details of input data formats are given in sections 3.2 and details of the output are given in section 3.3 of this chapter.

OPTION 0 should be employed with care and only if "real" climatological and field data are available, because the hydrologic parameters (e.g., rainfall vs. soil moisture content) are always correlated, though independency is assumed for these input data. This option has specialized applications such as: ~~screening of~~ comparing a large number of chemicals that are to be compared for their environmental effects when released into non-site specific (scenario) soil compartments. (Bonazountas et al 1982).

3.1.4.3 OPTION A -- Annual Simulation; Estimated Water Balance

OPTION A is philosophically like OPTION 0; however, it has been designed for region specific simulations, or for testing the importance of seasonality and the output of option M (Summary Report).


AIR COMPARTMENT
Precipitation
(Rain, Snow)
EVAPOTRANSPIRATION
SURFACE RUNOFF
Evaporation
Waste Disposal Site
Infiltration
Treatment Plant
Storage
UPPER UNSATURATED SOIL ZONE
SURFACE RUNOFF
LOWER UNSATURATED SOIL ZONE
Groundwater Recharge
Capillarity
SATURATED ZONE
Groundwater Recharge
GROUNDWATER RUNOFF
GROUNDWATER RUNOFF
Bedrock
WATER COMPARTMENT
STREAM
CHANNEL, ESTUARY

Participation

Main focus this version

Not modeled in this version

FIGURE 3-3 Compartment Disaggregation; OPTION O, OPTION A

The simulation is performed annually and for only one year and requires the knowledge of a few annual averaged climatic and soil data for the area, in order for the model to estimate the annual hydrologic (water balance) parameters relating to the compartment, which are user inputs to OPTION 0.

The user has to input: (1) climatic and storm parameters, (2) soil parameters which may vary in the two layers, (3) chemical parameters, (4) simulation specific parameters, and (5) washload parameters. These data are readily available from the literature (e.g., NOAA reports, handbooks).

The output from the model consists of: (1) the hydrologic cycle components of the annual compartmental water balance, (2) the washload from the compartment, (3) the annual pollutant distribution (e.g., concentrations, mass to groundwater).

As in OPTION 0, simulations are performed in two unsaturated soil zone layers (Figure 3-3), are performed annually and for only one year, and are of use for specialized applications. Additional information for this level is provided in Section PT-3.2. Details of input/output data formats are given in Sections 3.2 and 3.3.

3.1.4.4 OPTION M — Monthly Simulations; Estimated Water Balances

OPTION M resembles OPTION A philosophically; however, operations are performed monthly and up to four soil layers (Figure 3-4) may be employed. Up to 10 years can be simulated.

In contrast to the input data required by OPTION A, the user has to know: (1) the monthly distribution of rainfall depths and other climatic parameters in the area, and (2) the monthly distribution of input pollutant (pollutant mass) to the compartment. Most other input data are similar to OPTION A. The monthly output from the model resembles the OPTION A annual output.

Simulations performed with OPTION M may reflect site specificity, both in time (averages over month) and area (reflected in the compartment characteristics). Input data are easily compiled from existing data sources (e.g., NOAA, handbook, this documentation); however, for site specific simulations, model output has to be compared to actual field data (for both hydrology and chemistry), and should be calibrated. Validation of final output is essential (See section 3.4).

Additional information describing internal operation of this option is provided in section PT-3.3. Details of input/output data formats are given in Sections 3.2 and 3.3 of this user's manual.

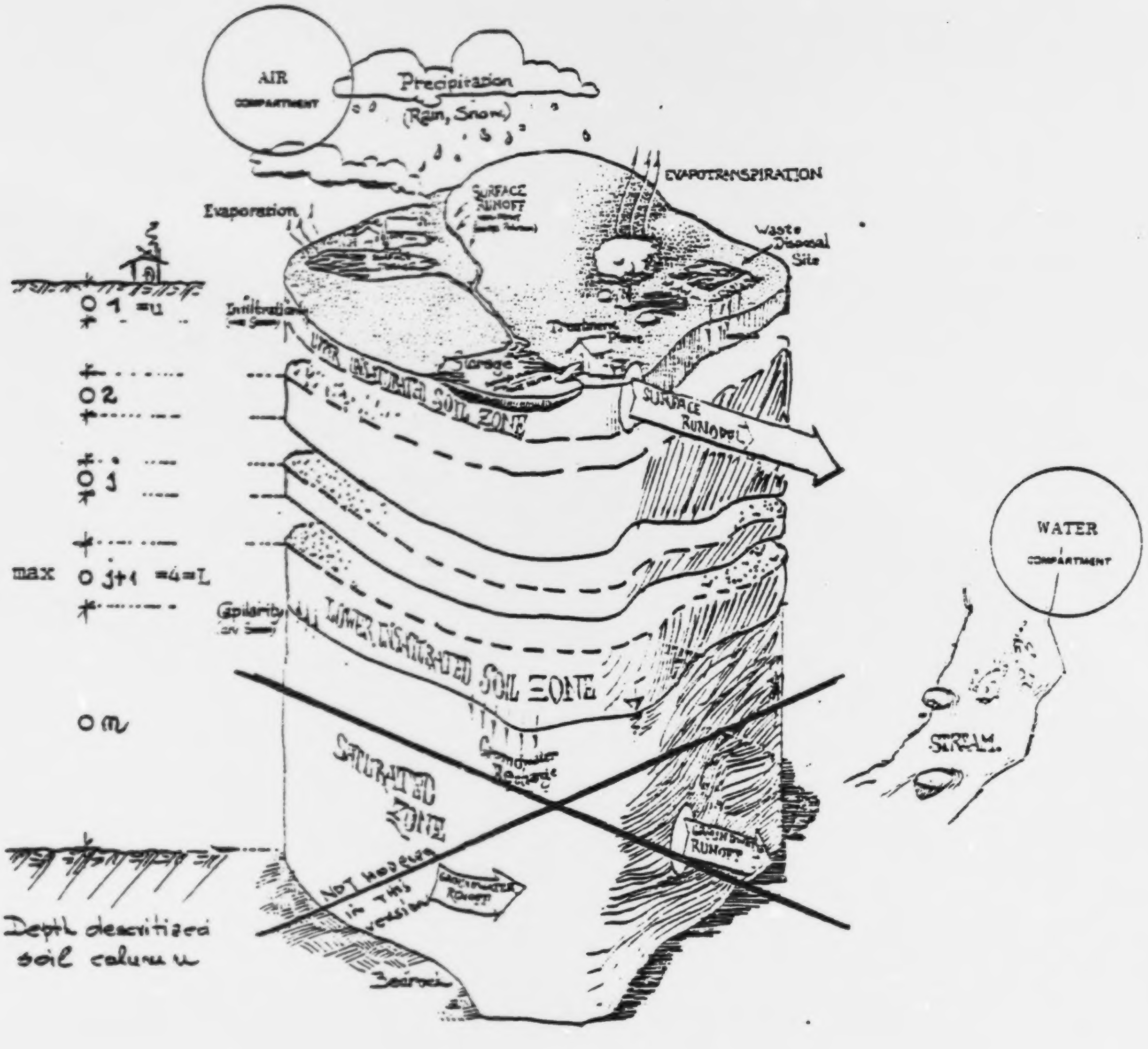

AIR COMPARTMENT
Precipitation
(Rain, Snow)
EVAPOTRANSPIRATION
Evaporation
SURFACE RUNOFF
Waste Disposal Site
Infiltration
Treatment Plant
Storage
UPPER UNSATURATED SOIL ZONE
SURFACE RUNOFF
O 1 =u
O 2
O j
max O j+1 =4=L
O m
Capillarity
LOWER UNSATURATED SOIL ZONE
Groundwater Recharge
SATURATED ZONE
GROUNDWATER RUNOFF
NOT modeled in this version
GROUNDWATER RUNOFF
Bedrock
Depth descritized soil column u
WATER COMPARTMENT
STREAM

FIGURE 3-4   Compartment Disaggregation; OPTION M

3.1.4.5 Other Options

It is possible to develop additional options, for example: a storm-by-storm temporal resolution and a N-layered compartment that may handle release of a second phase (insoluble) chemical spill on the soil surface. However, this has not been the focus of this version of SESOIL. A storm-by-storm version of SESOIL can be developed by designing, for example, a statistical disaggregation model for the rainfall record that will not require additional input data. Such SESOIL operational options can become part of future model capabilities.

3.1.5 Canonical/Scenario Chemical Fate Modeling

Recent concerns related to environmental quality require a methodology to relate sources and quantities of chemical released into the environment to the actual amounts of these chemicals to which humans and other biota are exposed (e.g., Bonazountas et al 1982). SESOIL is well suited for such overall environmental fate studies, which are based on "canonical" environmental compartments and employ typical scenarios (single medium or multimedia). It has to be emphasized that the selection (compilation) of canonical compartments is not an easy task and has to involve consideration of statistical techniques (e.g., kriging, see Section 3.4.3) to optimally (appropriately) design the compartments. Although no final methodology for the design of canonical environments has yet been developed, a preliminary logic for a scenario design will be presented (1985) in Appendix MI.

3.2 DATA STRUCTURE AND MANAGEMENT

3.2.1 General

This section is intended to give the user an overview of the:

(1) model program and data structure,
(2) content of the input data files, and
(3) model execution.

3.2.2 SESOIL Program and Data Structure

A generalized flow chart of SESOIL data files and operation is shown on Figure 3-5. The executive program of operations, designated as SE84, calls the main program designated as SESOIL, and the latter calls the two basic data subroutines RFILE (read data file), PFILE, and one of the two primary subroutines annual (OPTION A) or monthly (OPTION M). Subsequently, each of the basic operational routines calls a number of secondary routines such as HYDROA (annual hydrologic routine), HYDROM (monthly hydrologic routine), WASHA (annual washload routine), WASHM (monthly washload routine), TRANSA (annual pollutant transport routine), TRANSM (monthly pollutant transport routine), and LAYER (called from TRANSM for each soil layer). Finally, each of the secondary routines calls a variety of functional routines, as presented in Appendix FC (FORTRAN Code).

A major design objective of SESOIL is the efficiency of data management and the easy input of data. Data are read by the model from 7 data files. In the IBM system, data files are accessed via the file name and a "DATA" designation. All files are expandable in size. The data files are:

ANNUAL DATA (OPTION 0,A — All hydrological and application data)
CLIMAT DATA (OPTION M — Climatological data)
SOIL DATA (OPTION A,M — Soil property data)
CHEM DATA (OPTION A,M — Chemical property data)
WASH DATA (OPTION A,M — Washload routine related data)
APPLIC DATA (OPTION M — Site specific area/application data)
EXEC DATA (All options — Executive operation indices)

For annual simulations (OPTION 0 and OPTION A) the files ANNUAL DATA, SOIL DATA, WASH DATA, and CHEM DATA are used. For monthly simulations the files CLIMAT DATA, SOIL DATA, WASH DATA, CHEM DATA, AND APPLIC DATA are used. The file names are descriptive, thus the SOIL DATA file contains soil parameters, APPLIC DATA contains application parameters (depths, pollutant loading), etc. Detailed information is provided in Sections 3.2.4.1-3.2.4.6, and in Section 3.2.5.

EXEC DATA (see also Section 3.2.4.7) contains information for each execution of SESOIL, such as the desired option of operation, desired

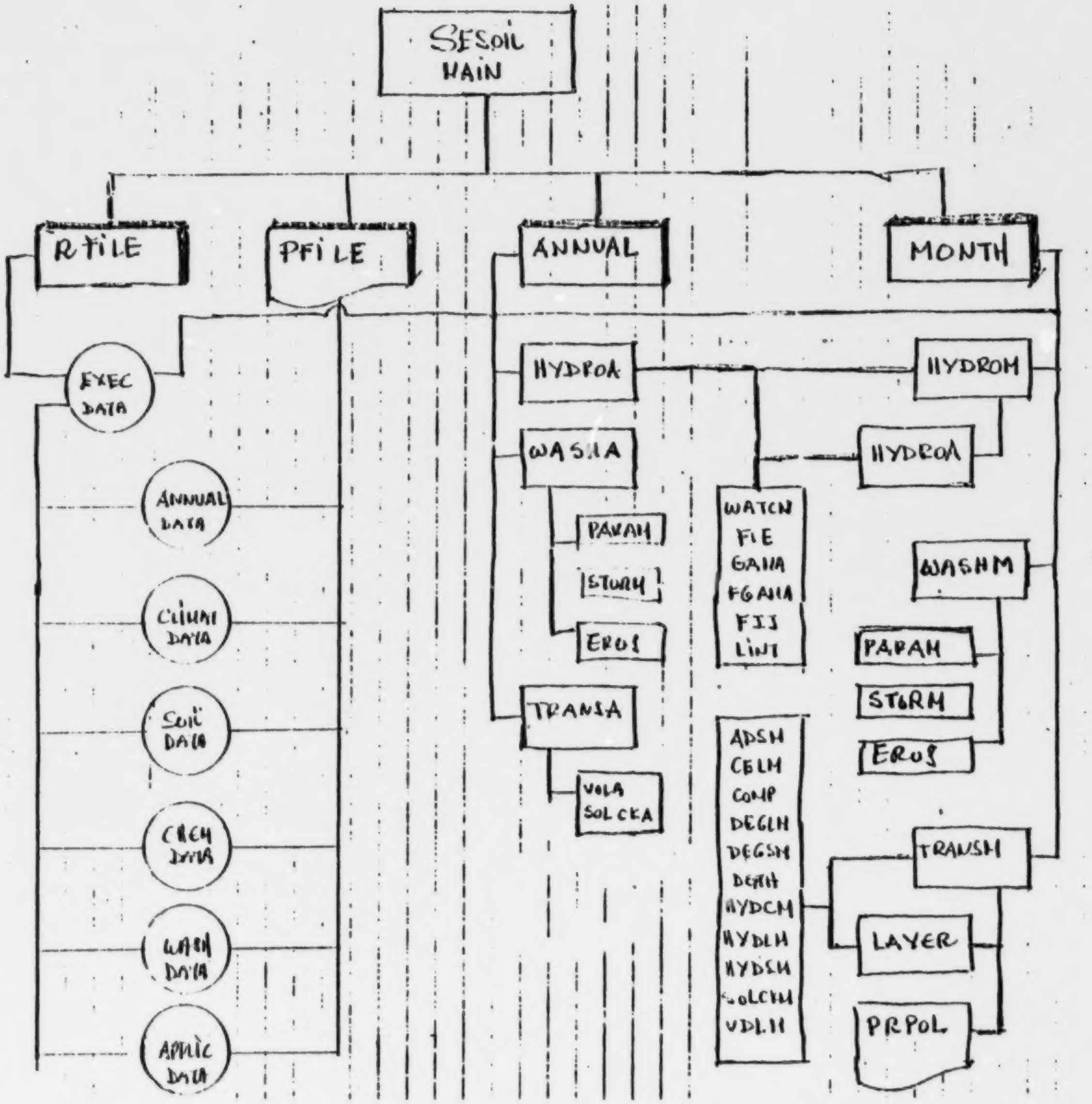

SESOIL MAIN
R FILE
PFILE
ANNUAL
MONTH
EXEC DATA
ANNUAL DATA
CLIMAT DATA
SOIL DATA
CHEM DATA
WASH DATA
APPLIC DATA
HYDROA
WASHA
PARAM
STORM
EROS
TRANSA
VOLA SOLCKA
WATCN
FIE
GAMA
FGAMA
FIJ
LINT
ADSM
CBLM
COMP
DEGLM
DEGSM
DEPTH
HYDCM
HYDLM
HYDSM
SOLCLM
VDLM
HYDROM
HYDROA
WASHM
PARAM
STORM
EROS
TRANSM
LAYER
PRPOL

FIGURE 3-5 Overview of Major Subroutines and Data Files

climatic area of simulation, and the desired type of soil or chemical compound. This file is used for both annual and monthly simulations.

Detailed information regarding the "loading" of these files is presented in Section 3.2.4 and in Appendix DF (Data Files).

3.2.3 Model Execution Philsophy

Model execution is accomplished with the following steps:

(1) The SESOIL user selects/decides on an option of operation (OPTION O, OPTION A, OPTION M).

(2) The user "edits" his basic data files (4 to 7 files, see section below)

- either through an interactive process via a screen terminal (e.g., IBM VM-CMS system), or
- by inserting or changing computer cards from his deck.

Editing of the basic data files involves either the input of new values (e.g., new climatological data) in the data files, or the updating of the previous information (e.g., another region).

Above files have unlimited expansion capabilities so that data from previous simulations may be saved for future comparative runs.

(3) The user asks for program execution via command appropriate to his computer system (e.g., SE84).

3.2.4 Input Data Files

The following 7 sections (3.2.4.1-3.2.4.7) give the information contained in, and formats of the 7 data files:

ANNUAL DATA	File of hydrologic and application information to be employed for annual simulations
CLIMAT DATA	File containing climatological data for monthly executions
SOIL DATA	File containing soil data for all executions
CHEM DATA	File containing chemical data for all executions
APPLIC DATA	File containing application data for monthly executions

WASH DATA	File containing washload data for all simulations
EXEC DATA	Exec data file for all executions

The following symbols are used in this documentation:

*****	indicates repetition of data lines or data sets
!!!!!	indicates important comments

Please note that SESOIL data files are formatted and thus data must be entered in the appropriate columns, with decimals if real numbers, right justified if integers, etc. Examples in the following sections will show some of the input files as coded for entry.

Section 3.2.5 presents a summary of all data entries for all files. Readers familiar with data entry may consult only that section.

3.2.4.1 ANNUAL DATA File

3.2.4.1.1 General

This file (Figure 3-6) contains application data and hydrologic or climatologic data applicable to both annual simulation options, OPTION 0 and OPTION A. This file is permanent and easily expandable.

Information contained in the file includes:

(1) Annual hydrologic data (water balance parameters) and washload mass for OPTION 0 simulations, or

(2) Annual climatologic data for OPTION A simulations,

(3) Application data for both annual options.

The user can input a series of data blocks of annual data in any sequence. The program can "spot" the correct data set via a user specified index (e.g., "3" SITE A (KANSAS); Figure 3-6). This index does not have to be sequentially numbered.

Only the numerical data is read by the program. Most of the other labels and text are designed for the user's aid. However, appropriate labeling and numbering is a good practice. The model is delivered with a small ANNUAL DATA file, so that labeling and formatting of new data can be done by example.

Section 3.2.5 presents a summary of all data entries for all files. Readers familiar with data entry may consult only that section.

```
    1 CLINTON, MA (SUB-HUMID)   OPTION A
 TA,NN,S,A,REP                   8.40   0.35   0.70   0.30   0.15
 MPA,MTR,MN,MT                  94.10   0.32 109.00 365.00
 THA,INF,RGA,RSA,WASHA
 AR,L,DU,DL,PHU,PHL              1.00  42.50   15.0  9985.   8.0    7.0
 AKDEL,AKDES,AOC,ACEC,AKOC       1.1    1.1    1.2   .001   1.0
 VOLU,ISRA,ASL                   0.5    0.40   0.40
 POLINU,POLINL,LIGU,LIGL        200.   1000.   10.   2000.
    2 CLINTON, MA (SUB-HUMID)   OPTION 0
 TA,NN,S,A,REP                   8.40
 MPA,MTR,MN,MT
 THA,INF,RGA,RSA,WASHA           9.76   67.43  19.03  35.12  0.09
 AR,L,DU,DL,PHU,PHL              1.00          15.0  9985.   8.0    7.0
 AKDEL,AKDES,AOC,ACEC,AKOC       1.1    1.1    1.2   .001   1.0
 VOLU,ISRA,ASL                   0.5    0.40   0.40
 POLINU,POLINL,LIGU,LIGL        200.   1000.   10.   2000.
    3 SITE A (KANSAS) (1940-1980) OPTION 0
 TA,NN,S,A,REP                  14.0
 MPA,MTR,MN,MT
 THA,INF,RGA,RSA,WASHA          11.06   85.0   16.5    0.0
 AR,L,DU,DL,PHU,PHL             10.0           15.   9985.   8.0    7.0
 AKDEL,AKDES,AOC,ACEC,AKOC       1.1    2.1    1.2    0.4   1.3
 VOLU,ISRA,ASL                   1.0    1.0   .497
 POLINU,POLINL,LIGU,LIGL       5000.   1000.   10.    50.
    4 SITE A (KANSAS) (1940-1980) OPTION A (USE KOC)
 TA,NN,S,A,REP                  14.0    .30    .60    .10
 MPA,MTR,MN,MT                  85.     .20   110.   365.
 THA,INF,RGA,RSA,WASHA
 AR,L,DU,DL,PHU,PHL             10.0   39.     15.   9985.   8.0    7.0
 AKDEL,AKDES,AOC,ACEC,AKOC       1.1    2.1    1.2    0.4   1.3
 VOLU,ISRA,ASL                   1.0    1.0   .497
 POLINU,POLINL,LIGU,LIGL       5000.   1000.   10.    50.
  999 END OF FILE
```

FIGURE 3-6 ANNUAL DATA File

3.2.4.1.2 ANNUAL Data Input

Data description, formats, and units for each line are described below. Sample values, from Figure 3-6 are also given for each line. The line numbers used below refer to Figure 3-6 and are employed for demonstration purposes only. These line numbers do not appear in the data file.

Line 1 FORMAT(2X,I3,1X,12A4)

Contains the heading of an area where the model may be applied

1 CLINTON, MA (SUB-HUMID) OPTION A

The above is not an executable statement. The number "1" before the area has to appear in the statement.

Line 2 FORMAT(38X,6F7.2)

For OPTION 0 this line contains the following data:

TA (^{o}C)	average annual temperature of area at surface (e.g., 8.40)

For OPTION A this line contains the following data:

TA (^{o}C)	average annual temperature of area at surface (e.g., 8.40)

- either

NN (fraction)	average annual fraction of sky covered by clouds (e.g., 0.35)
S (fraction)	average annual fractional relative humidity of the area (e.g., 0.70)
A (-)	average annual short wave albedbo of the surface (e.g., 0.15)

- or (if Known)

REP (cm/day)	average annual evapotranspiration rate of the area (e.g., 0.15)

- Set REP to 0 if wish to estimate it

"both" above sets can be given, if the user desires so; however, the program will assume the evapotranspiration rates in the area is "known" and will "not" estimate it from the first data set TA, NN, S, A.

Line 3 FORMAT (38X,4F7.2)

For OPTION 0 this line must be entered but should be left blank.

For OPTION A this line contains the following data:

MPA (cm)	annual depth of rain (e.g., 94.10)
MTR (day)	annual mean storm duration (e.g., 0.32)
MN (-)	number of storm events per year (e.g., 109.00)
MT (days)	mean length of rainy season (e.g., 365.0)

Line 4 FORMAT (38X,5F7.2)

FOR OPTION 0 this line contains the following data:

THA (-)	average annual soil moisture content (%) (e.g., 9.76)
IA (cm)	annual total infiltration (e.g., 67.43)
RGA (cm)	annual total groundwater recharge (e.g., 19.03) Assumed equivalent to groundwater runoff for these options.
RSA (cm)	annual total surface runoff (e.g., 35.12)
WASHA (ug/cm^2)	annual total washload loss (e.g., 0.09)

For OPTION A this line must be entered but should be left blank.

Line 5 FORMAT (38X,6F7.2)

For both options this line contains:

AR (cm^2)	surface area of the compartment (e.g., 1.00)
L (degrees)	latitude of the area (e.g., 42.50)
DU (cm)	depth of upper unsaturated soil zone for this application (e.g., 15.0)
DL (cm)	depth of lower unsaturated soil zone for this application (e.g., 9985.)

PHU (-)	pH of upper soil zone (e.g., 8.0)
PHL (-)	pH of lower soil zone (e.g., 7.0)

Note: Latitude is optional for OPTION 0. For OPTION 0 this field may be left blank.

Line 6 FORMAT (38X,5F7.2)

For both annual options this line contains the following data:

AKDEL (-)	ratio: biodegradation rate in liquid phase in lower soil zone to upper soil zone. (e.g., 1.1)
AKDES (-)	ratio: biodegradation rate on solid phase in lower soil zone to upper soil zone (e.g., 1.1)
ACC (-)	ratio: organic carbon content in soil in lower soil zone to upper soil zone (e.g., 1.2)
ACEC (-)	ratio: cation exchange capacity of soil in lower soil zone to upper soil zone (e.g., .001)
AKCC (-)	ratio: adsorption coefficient of soil in lower soil zone to upper soil zone (e.g., 1.0)

Line 7 FORMAT (38X,3F7.2)

VOLU (-) index of volatilization occurrance in upper soil zone (e.g., 1.0)

VOLU = 0 no volatilization from upper soil zone
VOLU = 1 volatilization allowed from upper soil zone
VOLU = 0.50 partial volatilization allowed (e.g. 0.5)

ISRA (-) Index of surface runoff pollutant transport (e.g., 0.40)

ISRA = 0 no pollutant transport in surface runoff
ISRA = 1 pollutant transport allowed in surface runoff

ISRA = 0.40 partial pollutant transport allowed

ASL (-)	ratio of pollutant concentration in rain to maximum solubility in water (e.g., 0.40)

Line 8 FORMAT (38X,4F7.2)

For both annual options this line contains the following data:

POLINU (ug/cm^2)	total pollution load (mass) per unit area (cm^2) per year, entering the compartment in the upper zone (e.g., 200.0)
POLINL (ug/cm^2)	total pollution load (mass) per unit area (cm^2) per year, entering the compartment in the lower zone (e.g., 1000.0)
LIGU (ug/cm^2)	ligand input mass to upper zone (ug/cm^2) (e.g., 10.00)
LIGL (ug/cm^2)	ligand input mass to lower zone (ug/cm^2) (e.g., 2000.0)

***** Above data set (lines 1-8) can be repeated for multiple sites in this data file (e.g., 2 CLINTON, MA (SUB-HUMID) OPTION O, etc.).

Line 25 FORMAT (2X,I3,39X)

The last line of this file indicates the end of the file as follows:

999 END OF FILE

3.2.4.2 CLIMAT DATA File

3.2.4.2.1 General

This file (Figure 3-7) contains climatologic data applicable to monthly simulations (OPTION M). This file is permanent and expandable.

Information contained in this file includes:

(1) Monthly climatologic data for a region (e.g., temperature, humidity)

```
   1 SITE A (KANSAS) 40 YR AVERAGES                          5
       ****  YEAR 1 ****
TA     14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3
NN      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
S       0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6
A       0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1
REP     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
MPM    6.40   4.22   2.95   2.46   3.20   5.20   7.82   11.1   12.2   9.97   10.2   9.12
MIR     0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2
MN     7.92   5.22   3.65   3.04   3.96   6.43   9.68   13.7   15.1   12.3   12.7   11.3
MT     30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5
       **** YEAR 2 ****
TA     14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3
NN      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
S       0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6
A       0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1
REP     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
MPM    6.40   4.22   2.95   2.46   3.20   5.20   7.82   11.1   12.2   9.97   10.2   9.12
MIR     0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2
MN     7.92   5.22   3.65   3.04   3.96   6.43   9.68   13.7   15.1   12.3   12.7   11.3
MT     30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5
       **** YEAR 3 ****
TA     14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3
NN      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
S       0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6
A       0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1
REP     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
MPM    6.40   4.22   2.95   2.46   3.20   5.20   7.82   11.1   12.2   9.97   10.2   9.12
MIR     0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2
MN     7.92   5.22   3.65   3.04   3.96   6.43   9.68   13.7   15.1   12.3   12.7   11.3
MT     30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5
       **** YEAR 4 ****
TA     14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3
NN      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
S       0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6
A       0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1
REP     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
MPM    6.40   4.22   2.95   2.46   3.20   5.20   7.82   11.1   12.2   9.97   10.2   9.12
MIR     0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2
MN     7.92   5.22   3.65   3.04   3.96   6.43   9.68   13.7   15.1   12.3   12.7   11.3
MT     30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5
       **** YEAR 5 ****
TA     14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3
NN      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
S       0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6
A       0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1
REP     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
MPM    6.40   4.22   2.95   2.46   3.20   5.20   7.82   11.1   12.2   9.97   10.2   9.12
MIR     0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2
MN     7.92   5.22   3.65   3.04   3.96   6.43   9.68   13.7   15.1   12.3   12.7   11.3
MT     30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5
   2 SITE A (KANSAS) TEST DATA EQUAL INPUT EACH MONTH        2
       ****  YEAR 1 ****
TA     14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3
NN      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
S       0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6
A       0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1
REP     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
MPM    10.0   10.0   10.0   10.0   10.0   10.0   10.0   10.0   10.0   10.0   10.0   10.0
MIR     0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2
MN     12.0   12.0   12.0   12.0   12.0   12.0   12.0   12.0   12.0   12.0   12.0   12.0
MT     30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5
       ****  YEAR 2 ****
TA     14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3   14.3
NN      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
S       0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6    0.6
A       0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1
REP     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
MPM    10.0   10.0   10.0   10.0   10.0   10.0   10.0   10.0   10.0   10.0   10.0   10.0
MIR     0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2    0.2
MN     12.0   12.0   12.0   12.0   12.0   12.0   12.0   12.0   12.0   12.0   12.0   12.0
MT     30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5   30.5
```

FIGURE 3-7   CLIMAT DATA File

(2) Monthly storm parameters for a region (e.g., depth of rain).

The user can input the data blocks of climatologic data in any sequence. The program can "spot" the correct data set via a user specified index (e.g., 1 SITE A (KANSAS), Figure 3-7). This index does not have to be sequentially numbered.

Only the numerical data is read by the program. Most of the other labels and text are designed for the user's aid. However, appropriate labeling and numbering is a good practice. SESOIL is delivered with a small CLIMAT DATA file, so that labeling and formatting of new data can be done by example.

Section 3.2.5 presents a summary of all data entries for all files. Readers familiar with data entry may consult only that section.

3.2.4.2.2 CLIMAT Data Input

Data descriptions, formats and units for each line are described below. Sample values, from Figure 3-7 are also given for each line. The line numbers used below refer to Figure 3-7 and are employed for demonstration purposes only. These line numbers do not appear in the data file.

Line 1 FORMAT (2X,I3,1X,12A4,I5)

Contains the heading of an area where the model may be applied:

```
1 SITE A (KANSAS) 40 YR AVERAGES      5
```

This line is not an executable statement. However, the numbers "1" and "5" must appear in the statement and in the correct columns. The "1" is the file index. The "5" is an index specifying the number of years of data in this data block. (5 years in Figure 3-7.)

Line 2 FORMAT (80X)

This line is used for separation and labeling purposes only. Any text may be entered on this line. (e.g., ***** YEAR 1 *****)

Lines 3 to 11 FORMAT (8X,12F6.2)

These lines contain the monthly values of the following parameters, starting with the October value in column 1 and ending with the following September value in column 12.

TA (°C)	average monthly temperature of the area (e.g., 14.3)
NN (fraction)	average monthly fraction of sky covered by clouds (e.g., 0.3)
S (fraction)	average monthly relative humidity of area (e.g., 0.6)
A (fraction)	average monthly shortwave albedo of the surface (e.g., 0.1)
REP (cm/day)	average daily evapotranspiration or 0.0
MPM (cm)	monthly precipitation depth (e.g., 6.40)
MTR (days)	mean time of rain (e.g., 0.2)
MN (-)	mean number of storm events (e.g., 7.92)
MT (days)	mean length of rain season (i.e. days in a month). If it rains at least 3-4 days in a week during the entire month, then MT=365/12=30.50 (e.g., 30.50)

Note: If evapotranspiration rate (REP) is entered as 0.0, this rate is calculated from previous parameters (TA, NN, S, and A). If evapotranspiration is entered as a non-zero value the NN, S and A values are ignored (and may be left blank).

***** The above lines (2-11) may be repeated for subsequent years for the same area. Up to 10 years of data may be entered per data set.

***** The above data set (lines 1-11) may be repeated for any number of areas by indexing (e.g., 2 SITE A (KANSAS) TEST..., Figure 3-7).

Line 105 FORMAT (2X,I3,39X)

The last line of this file indicates the end of file as follows:

999 END OF FILE

3.2.4.3 SOIL DATA File

3.2.4.3.1 General

This file (Figure 3-8) contains soil data applicable to all simulations. This file is permanent and expandable.

The user can input the data blocks of soil data in any sequence. The program can "spot" the correct data set via a user specified index (e.g., "1" CLAY, Figure 3-8). This index does not have to be sequentially numbered.

Only the numerical data is read by the program. Most of the other labels and text are designed for the user's aid. However, appropriate labeling and numbering is a good practice. The model is delivered with a small SOIL DATA file, so that labeling and formating of new data can be done by example.

Section 3.2.5 presents a summary of all data entries for all files. Readers familiar with data entry may consult only that section.

3.2.4.3.2 Data Input

Data descriptions, formats and units for each line are described below. Sample values, from Figure 3-8 are also given for each line. The line numbers used below refer to Figure 3-8 and are employed for demonstration purposes only. These line numbers do not appear in the data file.

Line 1 FORMAT (2X,I3,1X,12A4)

Contains the description of the indexed soil type whose data follow; e.g.

1 CLAY

Line 2 FORMAT (38X, 5F7.2)

This line contain the following data:

RS (g/cm^2)	soil bulk density (e.g., 1.32)
K1 (cm^2)	soil intrinsic permeability (e.g. 1.00 x 10^{-10})

```
1 CLAY
     -  RS,K1,C,N,OC                  1.32 1.E-10  12.00   0.45   1.46
     -  CEC,FRN                      15.00   1.4
2 SILTY-LOAM (KANSAS)
     -  RS,K1,C,N,OC                  1.32 .7E-08   6.00   0.35   2.9
     -  CEC,FRN                       0.00   1.4
3 SILTY-LOAM (KANSAS) (ANNUAL TEST)
     -  RS,K1,C,N,OC                  1.32 .7E-08   6.00   0.35   2.9
     -  CEC,FRN                       10.     1.4
4 SILTY-LOAM DEFAULT
     -  RS,K1,C,N,OC                  1.4 .35E-09   5.50   0.35   2.9
     -  CEC,FRN                       0.0     1.0
999 END OF FILE
```

FIGURE 3-8 SOIL DATA File

C (-)	soil disconnectedness index (see Appendix HY) (e.g. 12.00)
N (-)	effective soil porosity (e.g. 0.45)
OC (%oc)	organic content of soil (e.g., 1.46)

Line 3 FORMAT (38X,2F7.2)

This line contains the following data:

CEC (me/100 g soil)	cation exchange capacity (e.g., 15.00)
FRN (-)	Freundlich equation exponent (e.g., 1.4)

Note: FRN is used only in monthly (OPTION M) simulations. For OPTION O and OPTION A simulations this field may be left blank.

***** The above data set (Lines 1-3) may be repeated for any number of soil types by indexing (e.g., 2 SILTY-LOAM (KANSAS), Figure 3-8).

Line 13 FORMAT (2X,I3,39X)

The last line of this file indicates the end of file as follows:

999 END OF FILE

3.2.4.4 CHEM DATA File

3.2.4.4.1 General

This file (Figure 3-9) contains chemical data applicable to all simulation options. This file is permanent and expandable.

Reference temperature appropriate (approximately annual average for soil process is left to the user.

The user can input the data blocks of chemical data in any sequence. The program can "spot" the correct data set via a user specified index (e.g., "1" 1,1-TRICHLOROETHANE (TCE) Figure 3-9). This index does not have to be sequentially numbered.

```
1 1,1-TRICHLOROETHANE (TCE)
    - SL,DA,H,KOC,K                1100.00  0.04 3.93E-3 180.00   0.00
    - MWT,VAL,KNH,KBH,KAH           133.4   0.00   0.00    0.00   0.00
    - KDEL,KDES,SK,B,MWTLIG           0.00  0.00   0.00    0.00   0.00
2 TEST CHEM (USE KOC)
    - SL,DA,H,KOC,K                   1.57 8.3E-6 9.4E-3   6.00   0.00
    - MWT,VAL,KNH,KBH,KAH             5.00  6.00 7.0E-6    8.00   9.00
    - KDEL,KDES,SK,B,MWTLIG           0.22  0.19 1.0E-5    3.30   4.40
3 1,1-TRICHLOROETHANE (KANSAS TEST)
    - SL,DA,H,KOC,K                1100.00  .083  .0094  360.00   0.00
    - MWT,VAL,KNH,KBH,KAH             0.00  0.00   0.00    0.00   0.00
    - KDEL,KDES,SK,B,MWTLIG           0.00  0.00   0.00    0.00   0.00
999 END OF FILE
```

FIGURE 3-9 CHEM DATA File

Only the numerical data is read by the program. Most of the other labels and text are designed for the user's aid. However, appropriate labeling and numbering is a good practice. The model is delivered with a small CHEM DATA file, so that labeling and formating of new data can be done by example.

Section 3.2.5 presents a summary of all data entries for all files. Readers familiar with data entry may consult only that section.

3.2.4.4.2 CHEM Data Input

Data descriptions, formats and units for each line are described below. Sample values, from Figure 3-9 are also given for each line. The line numbers used below refer to Figure 3-9 and are employed for demonstration purposes only. These line numbers do not appear in the data file.

Line 1 FORMAT (2X,I3,1X,12A4)

Contains the description of the indexed chemical compound type whose data follow: e.g.

1 1,1 TRICHLORETHANE (TCE)

Line 2 FORMAT (38X,5F7.2)

This line contains the following data:

SL (ug/mL)	compound solubility in water (e.g., 1100)
DA (cm^2/sec)	diffusion coefficient in air (e.g., 0.04)
H (m^3.atm/ °K.mol)	Henry's law constant (e.g., 3.93E-3)
KOC (ug/goc)/ (ug/mL)	adsorption coefficient of the compound on organic carbon (e.g., 180.00)
K (ug/g)/ (ug/mL)	averaged adsorption coefficient for the compound on the soil (e.g., 0.0)

Note: If a nonzero value is entered for K, the program will use this value as an adsorption coefficient. Otherwise, KOC will be used.

Line 3 FORMAT (38X,5F7.2)

This line contains the following data:

MWT (g/mol)	molecular weight of compound (e.g., 133.4)
VAL (-)	valence of compound (e.g., 0.00)
KNH (day^{-1})	neutral hydrolysis constant (e.g., 0.00)
KBH (L/mol.day)	base catalyzed hydrolysis constant (e.g., 0.00)
KAH (L/mol.day)	acid catalyzed hydrolysis constant (e.g., 0.00)

Line 4 FORMAT (38X,5F7.2)

This line contains the following data:

KDEL (day^{-1})	biodegradation rate of compound in liquid phase (e.g., 0.00)
KDES (day^{-1})	biodegradation rate of compound in solid phase (e.g., 0.00)
SK (-)	stability constant of compound/ligand complex (e.g., 0.00)
B (-)	number of moles of ligand per mole of compound complexed (e.g., 0.00)
MWTLIG (g/mol)	molecular weight of ligand (e.g., 0.00)

***** The above data set (Lines 1-4) may be repeated for any number of compounds by indexing. (e.g., 2 TEST CHEM, Figure 3-9).

Line 13 FORMAT (2X,I3,39X)

The last line of this file indicates the end of file as follows:

999 END OF FILE

3.2.4.5 APPLIC DATA File

3.2.4.5.1 General

This file (Figure 3-10) contains application data applicable to monthly simulations (OPTION M). This file is permanent and expandable.

Information contained in this file includes:

(1) Site description (depths of layers, pH's, etc.)

(2) Soil and chemical parameters by soil zone.

(3) Pollutant loadings

The user can input the data blocks of application data in any sequence. The program can "spot" the correct data set via a user specified index (e.g., "1" TEST RUN, Figure 3-10). This index does not have to be sequentially numbered.

Only the numerical data is read by the program. Most of the other labels and text are designed for the user's aid. However, appropriate labeling and numbering is a good practice. The model is delivered with a small APPLIC DATA file, so that labeling and formatting of new data can be done by example.

Section 3.2.5 presents a summary of all data entries for all files. Readers familiar with data entry may consult only that section.

3.2.4.5.2 APPLIC Data Input

Data descriptions, formats and units for each line are described below. Sample values, from Figure 3-10 are also given for each line. The line numbers used below refer to Figure 3-10 and are employed for demonstration purposes only. These line numbers do not appear in the data file.

Line 1 FORMAT (2X,I3,1X,12A4)

Contains the description of the application area whose data follow; e.g.

1 TEST RUN

Line 2 FORMAT (38X,4F7.2)

This line contains the following data:

ILYS (-) number of soil layers to be simulated for application area (e.g., 4)

```
   1 TEST RUN
  -ILYS,IYRS,AR,L                                4.0    2.0   10.0    39.
  -D1,D2,D3,DL                                   15.    12.   10.0  4863.
  -PH1,PH2,PH3,PHL                               8.0    8.0    8.0    7.0
  -K11,K12,K13,K1L
  -KDEL MULTIPLIERS                              1.0    1.0    1.1
  -KDES MULTIPLIERS                              1.0    1.0    1.1
  -OC MULTIPLIERS                                1.0    1.0    1.2
  -CEC MULTIPLIERS                               0.1    0.1    0.1
  -FRN MULTIPLIERS                               1.0    1.0    1.0
  -ADS MULTIPLIERS                               1.0    1.0    1.0
                 **** LAYER 1 **  YEAR 1 ****
POLIN1 500.0  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS1  1.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK1   3.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG1   10.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF1   1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00
ISRM    0.20  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
ASL     0.10  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
                 **** LAYER 2 **  YEAR 1 ****
POLIN2  50.0  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS2  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK2   4.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG2   5000.  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
                 **** LAYER 3 **  YEAR 1 ****
POLIN3  50.0  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS3  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK3   4.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG3   5000.  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
                 **** LAYER 4 **  YEAR 1 ****
POLINL  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANSL  2.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINKL   4.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIGL   5000.  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLFL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
                 **** LAYER 1 **  YEAR 2 ****
POLIN1  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS1  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK1   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG1    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF1   1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00
ISRM    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
ASL     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
                 **** LAYER 2 **  YEAR 2 ****
POLIN2  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS2  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG2    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
                 **** LAYER 3 **  YEAR 2 ****
POLIN3  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS3  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG3    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
                 **** LAYER 4 **  YEAR 2 ****
POLINL  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANSL  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINKL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIGL    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLFL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
```

ange

FIGURE 3-10 APPLIC DATA File

```
  2 TEST RUN (2)
 -ILYS,IYRS,AR,L                                    2.0     1.0    10.0     39.
 -D1,DL                                            15.  4885.0
 -PH1,PHL                                           8.0     7.0
 -K11,K1L
 -KDEL MULTIPLIER                                   1.1
 -KDES MULTIPLIER                                   1.1
 -OC MULTIPLIERS                                    1.2
 -CEC MULTIPLIERS                                   0.1
 -PRN MULTIPLIERS                                   1.0
 -ADS MULTIPLIERS                                   1.0
                **** LAYER 1 **  YEAR 1 ****
POLIN1 500.0  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANS1  1.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINK1   3.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIG1   10.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLF1   1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00
ISRM    0.20  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
ASL     0.10  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
                **** LAYER 2 **  YEAR 1 ****
POLINL  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANSL  2.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINKL   4.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIGL   5000.  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
VOLFL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
 999 END OF FILE
```

FIGURE 3-10 (Cont.) APPLIC DATA File

IYRS (-)	number of years of data included in this data set (e.g., 2.0)
AR(cm^2)	surface area of the compartment (e.g., 10.0)
L (degrees)	latitude of the area (e.g., 39.0)

Lines 3-5 FORMAT (38X,4F7.2)

These lines contain parameters which characterize each soil layer. Each line will contain 2, 3, or 4 columns of data, depending on the number of layers specified in line 2. The first column contains the top layer's parameters, the following columns should refer to the lower layers in order of increasing depth.

DEPTH (cm)	depth of each layer
PH (-)	pH of each layer
K1 (-)	intrinsic permeability of each layer

Lines 6-11 FORMAT (38X,4F7.2)

These lines contain, for various soil and chemical parameters, the ratio of this parameter in a lower soil zone to the upper soil zone. Each line will contain 1, 2, or 3 columns of data, depending on the number of layers specified in line 2. The columns refer to the 2nd, 3rd, and 4th layer's ratios (in order of increasing depth). Note, each ratio is to the upper soil zone.

	KDEL Multipliers (-)	ratios for biodegradation in liquid phase
	KDES Multipliers (-)	ratios for biodegradation in solid phase
	OC Multipliers (-)	ratios for organic carbon content of soil
	CEC Multipliers (-)	ratios for cation exchange capacity in soil
to change	FRN Multipliers (-)	ratios for Freundlich exponent
	ADS Multipliers (-)	ratios for adsorption coefficient

Line 12 FORMAT (80X)

This line is used for separation and labeling purposes only. Any text may be entered on this line. (e.g., **** LAYER 1 * YEAR 1 ***).

Lines 13-19 FORMAT (8X,12F6.2)

These lines contain the monthly values of the following parameters, starting with the October value in column 1 and ending with the following September value in column 12.

POLIN1 (ug/cm^2)	monthly pollutant load (mass per unit area) entering the upper soil zone
TRANS1 (ug/cm^2)	monthly mass of pollutant transformed in the upper soil zone by processes not otherwise included in the model
SINK1 (ug/cm^2)	monthly mass of pollutant removed from the upper soil zone by processes not otherwise included in the model
LIG1 (ug/cm^2)	monthly ligand input mass to the upper soil zone
VOLF1 (-)	index of volatization occurance from the upper soil zone VOLF1=0 no volatilization from upper soil zone VOLF1=1 volatilizatoin allowed from upper soil zone
ISRM (-)	index of surface runoff pollutant transport ISRM=0 no pollutant transport in surface runoff ISRM=1 pollutant transport allowed in surface runoff
ASL (-)	ratio of pollutant concentration in rain to maximum solubility in water

Line 20 FORMAT (80X)

This line is used for separating and labeling purposes only. Any text may be entered on this line (e.g., **** LAYER 2** YEAR 1 *****)

Lines 21-25 FORMAT (8X,12F6.2)

These lines contain the monthly values of the following parameters, starting with the October value in Column 1 and ending with the following September value in Column 12.

POLIN2 (ug/cm^2)	monthly pollutant load (mass per unit area) entering the second soil zone
TRANS2 (ug/cm^2)	monthly mass of pollutant transformed in the second soil zone by processes not otherwise included in the model
SINK2 (ug/cm^2)	monthly mass of pollutant removed from the second soil zone by processes not otherwise in the model
LIG2 (ug/cm^2)	monthly ligand input mass to the second soil zone
VOLF2 (-)	index of volatilization occurance from the second soil zone VOLF2=0 no volatilization from second soil zone VOLF2=1 volatilization allowed from second soil zone

***** Lines 21-25 are repeated for each soil zone below the surface.

***** Lines 12-25 are repeated for each year specified in Line 1. Up to 10 years of data can be input per data set.

***** Above data set (Lines 1-25) can be repeated for multiple application areas by indexing (e.g., 2 TEST RUN (2), Figure 3-10)

Line 90 FORMAT (2X,I3,39X)

The last line of the file indicates the end of file as follows:

999 END OF FILE

3.2.4.6 WASH DATA File

3.2.4.6.1 General

This file (Figure 3-11) contains washload data applicable to all simulation options. This file is permanent and easily expandable.

The user can input the data blocks of washload data in any sequence. The program can "spot" the correct data set via a user specified index (e.g., "1" Clinton, MA. WASHLOAD; Figure 3-11). This index does not have to be sequentially numbered.

Only the numerical data is read by the program. Most of the other labels and text are designed for the user's aid. However, appropriate labeling and numbering is a good practice. The model is delivered with a small WASH DATA file, so that labeling and formatting of new data can be done by example.

Section 3.2.5 presents a summary of all data entries for all files. Readers familiar with data entry may consult only that section.

3.2.4.6.2 Data Input

Data descriptions, formats, and units for each line are described below. Sample values, from Figure 3-11 are also given for each line. The line numbers used below refer to Figure 3-11 and are employed for demonstration purposes only. These line numbers do not appear in the data file.

Line 1 FORMAT (2X,I3,1X,12A4,I5)

Contains the description of the indexed washload data set whose data follow; e.g., 1 CLINTON, MA. WASHLOAD 1

This line is not an executable statement. However, the numbers "1" and "1" must appear in the statement and in the correct columns. The first number is the file index. The second "1" is an index specifing the number of years of data in this data block.

Line 2 FORMAT (38X,6F7.2)

For both options this line contains the following data:

ARW(cm^2)	washload area (e.g., 1.E5)
SLT (fraction)	fraction of silt in the soil (e.g., 0.20)

```
  1 CLINTON,MA WASHLOAD                              1
  ARW,SLT,SND,CLY,SLEN,SLP           1.E5   0.20   0.66   0.14  6279. 0.0267

                 **ANNUAL DATA**
KSOIL   0.23
CFACT   0.26
PFACT   1.00
NFACT   0.03
  2 CLINTON,MA  (MONTHLY TIME STEP)                  2
  ARW,SLT,SND,CLY,SLEN,SLP           1.E5   0.20   0.66   0.14  6279. 0.0267

                 **MONTHLY DATA**  YR 1
KSOIL   0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23 0.23
CFACT   0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26 0.26
PFACT   1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00 1.00
NFACT   0.03  0.03  0.03  0.03  0.03  0.03  0.03  0.03  0.03  0.03  0.03 0.03
                 **MONTHLY DATA**  YR 2
KSOIL   0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23  0.23 0.23
CFACT   0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26  0.26 0.26
PFACT   1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00 1.00
NFACT   0.03  0.03  0.03  0.03  0.03  0.03  0.03  0.03  0.03  0.03  0.03 0.03
 999 END OF FILE
```

FIGURE 3-11 WASH DATA File

SND (fraction)	fraction of sand in the soil (e.g., 0.66)
CLY (fraction)	fraction of clay in the soil (e.g., 0.14)
SLEN (cm)	slope length of representative overload flow profile (e.g., 6279)
SLP (cm/cm)	average slope of representative overload flow profile (e.g., 0.026)

Note: SLT, SND, and CLY should add up to 1.0.

Line 3 FORMAT (80X)

This line is used for separation and labeling purposes only. Any text may be entered on the line (e.g., **ANNUAL DATA**).

Line 4 FORMAT (8X,12F6.2)

These lines contain the values of the following parameters. For monthly simulations all twelve columns must be entered, starting with the October value in column 1 and ending with the following September value in column 12. For annual simulations only column 1 should be entered, and columns 2-12 may be left blank.

KSOIL (tons/acre/English EI)	soil erodibility factor for slope (e.g., 0.23)
CFACT (-)	soil loss ratio for slope (e.g., 0.26)
PFACT (-)	contouring factor for slope (e.g., 1.0)
NFACT (-)	Manning's n for slope (e.g., 0.03)

***** The above (lines 3-4) may be repeated for subsequent years for the same area. Up to 10 years of data may be entered per data set.

***** The above data set (lines 1-4) may be repeated for any number of data sets by indexing (e.g., 2 Clinton, MA., Figure 3-11).

Line 20 FORMAT (2X,I3,39X)

The last line of this file indicates the end of file as follows:

999 END OF FILE

3.2.4.7 EXEC DATA File

This file (Figure 3-12) is used with all simulation options and controls the execution of the program, as well as the reading of the various data files. As such, EXEC DATA is employed in conjunction with one or more of the previously described data files.

After the first line, (which is used only for labeling purposes), each line of the EXEC DATA file corresponds to one run of SESOIL. An unlimited number of runs can be specified. Each line of the file contains 8 parameters (Figure 3-12). Format and description of these parameters are as follows:

Line 1 FORMAT (80X)

Any text can be used on this line, however, the following header is supplied as a guide to the file contents and format

RUN OPTN CLIM SOIL CHEM WASH APPL YRS

Line 2 FORMAT (I5,4X,A1,6I5)

This line contains the following execution parameters:

RUN (-)	incremental number of the run (i.e., 1,2, - - -)
OPTN (-)	simulation option (e.g., O, A, or M)
ANNUAL/CLIM (-)	For Option O and A: Index for annual data (e.g., 1 CLINTON, MA., from data file ANNUAL data) For Option M index for climatogic data (e.g., 1 for CLINTON, MASS from data file CLIMAT DATA)
SOIL (-)	index for soil data (e.g., 1 for CLAY)
CHEM (-)	index for chemical data (e.g., 1 for TCE)

```
RUN OPTN CLIM SOIL CHEM WASH APPL  YRS
  1    A    1    1    1    1    1    2
999 END OF FILE
```

<u>FIGURE 3-12</u> EXEC DATA File

WASH (-)	Index for washload data (e.g., 1 for CLINTON, WASHLOAD), 0 if omitted
APPL (-)	index for application area (e.g., 1 for TEST RUN)
YRS (-)	number of years to be simulated (e.g., 1-10)

*****	Multiple runs are specified with multiple run/line entries.
END OF FILE	The number 999 [FORMAT(I5)] indicates end of file.

3.2.5 Summary of Data Input

Table 3-1 summarizes all input data of the ANNUAL DATA file.

Table 3-2 summarizes all input data of the CLIMAT DATA file.

Table 3-3 summarizes all iput data of the SOIL DATA file.

Table 3-4 summarizes all input data of the CHEM DATA file.

Table 3-5 summarizes all input data of the WASH DATA file.

Table 3-6 summaries all input data of the APPLIC DATA file.

Table 3-7 summarizes all input data of the EXEC DATA file.

Note: Only 1 region, 1 soil type, 1 chemical, 1 washload set, and 1 application area are shown in the following tables. Following his familiarization with SESOIL, the user may consider consulting only the following tables to load data.

TABLE 3-1 ANNUAL DATA File
(Overview)

LINE	INPUT PARAMETERS/VARIABLES	FORTRAN Format
1	1 REGIONAL TITLE	2X,I3,1X,12A4
2	TA NN S A REP	38X,5F7.2
3	MPA MTR MN MT	38X,4F7.2
4	THA INF RGA RSA WASHA	38X,5F7.2
5	AR L DU DL PHU PHL	38X,6F7.2
6	AKDEL AKDES AOC ACEC AKOC	38X,5F7.2
7	VOLU ISRA ASL	38X,3F7.2
8	POLINU POLINL LIGU LIGL	38X,4F7.2
25	999 END OF FILE	2X,I3,39X

TABLE 3-2 CLIMAT DATA File (Overview)

LINE		INPUT PARAMETERS/VARIABLES		FORTRAN Format
1	1	REGIONAL TITLE	IYRS	2X,I3,1X,12A4,I5
2		LABEL		80X
3		TA (OCT)	TA (SEP)	8X,12F6.2
4		NN (OCT)	NN (SEP)	8X,12F6.2
5		S (OCT)	S (SEP)	8X,12F6.2
6		A (OCT)	A (SEP)	8X,12F6.2
7		REP(OCT)	REP(SEP)	8X,12F6.2
8		MPM(OCT)	MPM(SEP)	8X,12F6.2
9		MTR(OCT)	MTR(SEP)	8X,12F6.2
10		MN (OCT)	MN (SEP)	8X,12F6.2
11		MT (OCT)	MT (SEP)	8X,12F6.2
105	999	END OF FILE		2X,I3,39X

TABLE 3-3 SOIL DATA File (Overview)

LINE		INPUT PARAMETERS/VARIABLES	FORTRAN Format
1	1	SOIL TITLE	2X,I3,1X,12A4
2		RS K1 C N OC	38X,5F7.2
3		CEC FRN	38X,2F7.2
13	999	END OF FILE	2X,I3,39X

TABLE 3-4 CHEM DATA File (Overview)

LINE	INPUT PARAMETERS/VARIABLES	FORTRAN Format
1	1 CHEMICAL TITLE	2X,I3,1X,12A4
2	SL DA H KOC K	38X,5F7.2
3	MWT VAL KNH KBH KAH	38X,5F7.2
4	KDEL KDES SK B MWTLIG	38X,5F7.2
13	999 END OF FILE	2X,I3,39X

TABLE 3-5 WASH DATA File
(Overview)

LINE	INPUT PARAMETERS/VARIABLES	FORTRAN Format
1	1 WASHLOAD DATA TITLE	2X,I3,1X,12A4
2	ARW SLT SND CLY SLEN SLP	38X,6F7.2
3	LABEL	80X
4	KSOIL(OCT).............KSOIL(SEP)	8X,126.2
5	CFACT(OCT).............CFACT(SEP)	8X,126.2
6	PFACT(OCT).............PFACT(SEP)	8X,126.2
7	NFACT(OCT).............NFACT(SEP)	8X,126.2
20	999 END OF FILE	2X,I3,39X

TABLE 3-6 APPLIC DATA File
(Overview)

LINE	INPUT PARAMETERS/VARIABLES	FORTRAN Format
1	1 APPLICATION TITLE	2X,I3,1X,12A4
2	ILYS IYRS AR L	38X,4F7.2
3	D1 D2 D3 DL	38X,4F7.2
4	PH1 PH2 PH3 PHL	38X,4F7.2
5	K11 K12 K13 K1L	38X,4F7.2
6	KDEL MULTIPLIERS	38X,4F7.2
7	KDES MULTIPLIERS	38X,4F7.2
8	OC MULTIPLIERS	38X,4F7.2
9	CEC MULTIPLIERS	38X,4F7.2
10	FRN MULTIPLIERS	38X,4F7.2
11	ADS MULTIPLIERS	38X,4F7.2
12	LABEL	80X
13	POLIN1(OCT)....................POLIN1(SEP)	8X,12F6.2
14	TRANS1(OCT)....................TRANS1(SEP)	8X,12F6.2
15	SINK1 (OCT)....................SINK1 (SEP)	8X,12F6.2
16	LIG1 (OCT)....................LIG1 (SEP)	8X,12F6.2
17	VOLF1 (OCT)....................VOLF1 (SEP)	8X,12F6.2
18	ISRM (OCT)....................ISRM (SEP)	8X,12F6.2
19	ASL (OCT)....................ASL (SEP)	8X,12F6.2
20	LABEL	80X
21	POLIN2(OCT)....................POLIN2(SEP)	8X,12F6.2
22	TRANS2(OCT)....................TRANS2(SEP)	8X,12F6.2
23	SINK2 (OCT)....................SINK2 (SEP)	8X,12F6.2
24	LIG2 (OCT)....................LIG2 (SEP)	8X,12F6.2
25	VOLF2 (OCT)....................VOLF2 (SEP)	8X,12F6.2
90	999 END OF FILE	2X,I3,39X

TABLE 3-7 EXEC DATA File (Overview)

LINE	INPUT PARAMETERS/VARIABLES	FORTRAN Format
1	LABEL	80X
2	RUN OPTN ANNUAL/CLIM SOIL CHEM WASH APPL YRS	I5,1X,A4,6I5
3	999 END OF FILE	2X,I3,39X

3.3 MODEL EXECUTION

3.3.1 Data Requirements

Data Input to SESOIL consists of adding to and editing the various data files as previously described. The following paragraphs give the minimum data requirements for each simulation option. (See Tables 3-1 through 3-7.)

OPTION 0

ANNUAL DATA	Lines 1-8
SOIL DATA	Lines 1-3
CHEM DATA	Lines 1-4
EXEC DATA	Lines 1-2

OPTION A

ANNUAL DATA	Lines 1-8
SOIL DATA	Lines 1-3
CHEM DATA	Lines 1-4
EXEC DATA	Lines 1-2

OPTION M

CLIMAT DATA	Lines 1-11
SOIL DATA	Lines 1-3
CHEM DATA	Lines 1-4
APPLIC DATA	Lines 1-28
EXEC DATA	Lines 1-2
WASH DATA	Lines 1-4

3.3.2 Execution Station

On the IBM system the user has to give the statement referring to the appropriate set of commands subh as SE84, via a terminal or a card to start the model execution. On the VAX/DEC system the command is @SE84.

3.3.3 Examples of Execution (Output)

The output is intended to be self explanatory. Presently it provides information on

(1) all simulation input data (application, climatic, chemical, soil, other) employed in a particular run/ execution

(2) the hydrologic cycle components (estimated or assumed in OPTION 0), and the monthly or annual pollutant cycle components in two to four simulated soil zones of the compartment

(3) washload estimates from the watershed

(4) pollutant concentrations (in soil-moisture, soil-air and adsorbed on soil) in the various soil zones modeled

(5) pollutant masses in the various phases and zones within the soil compartment and released to air and ground

(6) averaged and/or totaled behavior of above cycles over a year of monthly simulations.

The SESOIL code, as released is set up to perform several example runs. Thus, once SESOIL is installed the user can give the control statement such as SE84 and receive sample output.

A typical input/output example is presented in Appendix AP (Applications).

3.4 MODEL "VALIDATION"

3.4.1 General

Model output validation is essential to any modeling effort. However, model "validation" is a very broad term and may include model verification, and application, calibration, validation, sensitivity, uncertainty, error, and model capability analyses. The definition of these terms and the procedures needed to accomplish these objectives are discussed in the following sections.

3.4.2 Model Application

Once a verified model has been obtained, the model may be applied by:

(1) Choosing the physical situation (site) to be modeled;
(2) Compiling the data required by the model;
(3) Inputing the data and running the model;
(4) Evaluating the model output.

In a validation effort, the above steps are usually performed several times, in an iterative manner. A common procedure is to seek a "final" model output which is based on several calibrations, which is then "validated." This iterative procedure is discussed in the following sections.

Compilation of data is intended to be relatively straightforward for SESOIL, since SEOIL employs parameters with physical and/or chemical meanings. The temporal and spacial resolution of the application can be chosen from the options provided in SESOIL. The desired resolution should be determined with previous understanding of the problem to be modeled, desired use of output, and data availability.

Input data can be grouped into the categories: (1) climatological, (2) geographic, (3) chemical, (4) soil, (5) washload, and (6) other. Table 3-8 presents some parameters associated with each category. Input data can be compiled from:

- site specific investigations and analyses (e.g., leaching rates of pollutants, soil permeability);
- national data bases (e.g., climatological data from the NOAA); and
- other sources (e.g., diffusion rate of pollutants from handbooks).

Once SESOIL has been used to perform a simulation the output can be calibrated and/or validated as explained below. Some expected outputs from the SESOIL model are:

TABLE 3-8

Soil Quality Modeling: Major Descriptors

CLIMATE: e.g.

- Evapotranspiration
- Temperature
- Latitude
- Sunlight
- Plant Cover
- Humidity
- Cloud Cover

SOIL: e.g.

- Porosity
- Bulk Density
- Hydraulic Conductivity
- Permeability
- Adsorption Capacity
- Organic Carbon Content
- Clay Content

GEOGRAPHY: e.g.

- Slope
- Surface Storage
- Terrain
- Area Coordinates

SOURCES: e.g.

- Release Mechanism
- Patterns of Operation (continuous, batch)
- Locations

Note: For details see Appendix ID.

- temporal and spatial pollutant concentration distributions in soil-air, soil-moisture;
- temporal and spatial pollutant concentration distributions on soil particles and in the basin washload; and
- leachate (pollutant mass) migration from unsaturated soil zone to groundwater and to receiving washload basin.

3.4.3 Model Calibration

Calibration of a model is the process in which the various model parameters are redetermined in order to provide the "best" simulation of previously known physical observations.

Such data usually include:

- soil moisture, soil infiltration or percolation rates; and
- water levels at gauging stations on the basin.

As discussed in Appendix PT, unsaturated models are mathematically designed by:

- developing a flow (moisture movement) submodel,
- developing a washload (sediment) submodel,
- developing a pollutant fate submodel, and
- interfacing the above three submodels.

A calibration procedure, in the context of SESOIL, applies to the flow model part of a code and, therefore, is defined as "the effort (parameter estimation) towards a historical matching of the climate, soil and water balance of a basin."

The calibration procedure is often referred to as the "inverse problem." Methods of solving this problem are discussed in the literature. Table 3-9 lists a number of current research efforts that are oriented towards calibrating mainly groundwater models. The same techniques might be applied for unsaturated soil zone models, although unsaturated soil zone modeling is complicated and no single mathematical method can optimally be applied. The following general discussion presents the concept of calibration as applicable to the SESOIL model.

When performing simulations, two different systems are being compared: (1) soil column and (2) the (conceptual) model. Data are taken from the first system, say, on basin annual yield (Eagleson 1978), in order

TABLE 3-9

References of Current Research in Calibration/Validation Procedures for Soil/Groundwater Model

Aguado, E., N. Sitar, and I Remson (1977). Sensitivity Analysis in Aquifer Studies. Journal of Geophysical Research, Vol. 13, No. 4, p. 733.

Bachmat, Y. and A. Dax (1979). An Iterative Method for Calibrating a Multicell Aquifer Model. Water Resources Research.

Brakensiek, D.L. and C.A. Onstad (1977). Parameter Estimation of the Green and Ampt Infiltration Equation. Water Resources Research, Vol. 13, No. 6, pp. 1009.

Cooley, R.L. (1977) A Method of Estimating Parameters and Assessing Reliability for Models of Steady State Groundwater Flow. 1. Theory and Numerical Properties. Water Resources, Vol. 15, No. 3, pp. 603-617.

Cooley, R.L. and P.J. Sinclair (1976). Uniqueness of a Model of Steady-State Groundwater Flow. Journal of Hydrology, Vol. 31, pp. 245-269.

Delhomme, J.P. (1979). Spatial Variability and Uncertainty in Groundwater Flow Parameters: A Geostatistical Approach. Water Resources Research,, Vol. 15, No. 2, pp. 269-280.

Delhomme, J.P. (1978). Driging in the Hydrosciences. Advances in Water Resources, Vol. 1, No. 5, pp. 251-266.

Dettinger, M.D. and J.L. Wilson (1981). First Order Analysis of Uncertainty in Numerical Models of Grounwater Flow. 1. Mathematical Development. Water Resources Research, Vo. 17, No. 1, pp. 149-161.

Gambolati, G. and G. Volpi (1979). A Conceptual Deterministic Analysis of the Kriging Technique in Hydrology. Water Resources Research, Vol. 15, No. 3, pp. 625-629.

Haverkamp, R. and M. Vauclin (1979). A Note on Estimating Finite Difference Iterblock Hydraulic Conductivity Values for Transient Unsaturated Flow Problems. Water Resources Research, Vo. 15, No. 1, pp. 181.

Preceding page blank

TABLE 3-9 (continued)

Hayhoe, H.N. (1978). Study of the Relative Efficiency of Finite Difference and Galerkin Techniques for Modeling Soil-Water Transfer. Water Resources Research, Vol. 14, No. 1, p. 97.

Hefez, E., U. Shamir, and J. Bear (1975). Identifying the Parameters of an Aquifer Cell Model. Water Resources Research, Vol. 11, No. 6, p. 993.

Kohberger, R.C., D. Scavia, and J. W. Wilkinson (1978). A Method for Parameter Sensitivity Analysis in Differencial Equation Models. Water Resources Research, Vol. 14, No. 1, p. 25.

McElwee, C.D. and M.A. Yukler (1978). Sensitivity of Groundwater Models with Respect to Variations in Transmissivity and Storage. Water Resources Research, Vol. 14, No. 3, pp. 451-459.

Murty, V.V.N. and V.H. Scott (1977). Determination of Transport Model Parameters in Groundwater Aquifers. Water Research, Vol. 13, No. 6, pp. 941.

Navarro, A. (1977). A Modified Optimization Method of Estimating Aquifer Parameters. Water Resources Research, Vo. 13, No. 6, pp. 935.

Nutbrown, D.A. (1975). Identification of Parameters in a Linear Equation of Groundwater Flow. Water Resources Research, Vol. 11, No.4, pp. 581.

Sagar, G, S. Yakowitz, and L. Duckstein (1975). A Direct Method for the Identification of the Parameters of Dynamic Nonhomogeneous Aquifiers. Water Resources Research, Vol. 11, No, 4, pp. 563.

to calibrate the latter. Roughly speaking, the calibration procedure for the model consists of finding a parameter set (intrinsic permeability, porosity) that minimizes deviations between observed and calculated values of annual yields. Least square's deviation is one of the methods employed in the literature. Other methods are linear programming, quadratic programming, and dynamic optimization. The least square's criterion may be written as:

$$\text{Minimize} \sum_{i=1}^{n} \left[Y^{(x,y,t)}_{\text{observed}} - Y^{(x,y,t)}_{\text{calculated}} \right]^{2}_{i}$$

where i = 1, . . . n, and n is the number of observed yield values.

The statistical analysis of parameter estimates and model predictions are very promising areas of current research. The mathematics involved, unfortunately, tend to be rather advanced and may be beyond the scope or needs of this modeling effort. Many of the parameter estimation techniques require both initial estimates of the soil cell parameters and their statistical properties. This has stimulated an interest in obtaining the statistical properties directly from field data. One of the more promising procedures is "kriging," which is a stochastic interpolation technique (Delhomme 1979).

Calibration is not a single process, neither is it a process that can be completely designed a priori. As more data become available, the calibration process should be repeated leading to improved model parameters. A schematic of the proposed calibration procedure is shown in Figure 3-13.

Calibration of unsaturated soil zone models can be uncertain and difficult because climate, soil moisture, soil infiltration and percolation are strongly interrelated parameters that can be difficult and/or expensive to measure in the field. Therefore, calibration of unsaturated soil zone models is frequrently associated with a model validation (described in the next section).

For the available version of SESOIL that employs Eagleson's (1978) annual water balance theory (as expanded to montly simulations and with moisture transfer budget in the course of the months), authors recommend model calibration by varying the intrinsic permeability (k), the pore disconnectedness index (c) and the porosity (n) of the soil. Other input parameters of the model can of course also be used to calibrate the model.

3.4.4 Model Validation

Frequently, the definitions of calibration and validation are synonymously employed in the literature because of the large number of nonvalidated but calibrated groundwater models and the limited number of noncalibrated but validated unsaturated soil zone models. For SESOIL, model validation is defined as "the process which analyses the validity of final model output." In SESOIL, validity is established by comparing the predicted pollutant concentrations to available knowledge of measured pollutant concentrations from monitoring data (field sampling).

A disagreement in absolute levels of concentration (predicted versus measured) does not necessarily indicate that either method of obtaining data (modeling, field sampling) is incorrect or that either data set needs revision. Field sampling approaches and modeling approaches rely on two different perspectives of the same situation.

Field data give concentrations at points in time and space. Models predict "average" concentrations for a particular assemed set of conditions. Thus, field and model results may differ and still both be correct. Some possible reasons for a discrepancy are:

- The field sample was taken from a spot with atypical concentrations (e.g., a water sample may be close to an unidentified confounding source,a nd so give abnormally high readings).

- The sample was taken under atypical conditions (e.g., on the one day/month that it rained); model results were calculated for average conditions, which may rarely occur (e.g., at the "average" soil moisture content which occurred only for a short period).

- The sample contained interactive compounds (e.g., a water sample contained some sodium that may have resutled in increased soil permeabilities).

- The extraction procedure for the sample was under or over efficient (e.g., it not only extracted all organic pollutants from a soil sample but also dissolved the soil).

Mathematically, the available model validation procedures and techniques are similar to those presented in the previous section. Following a validation procedure with good field data, "no better model predictions" can be made. This will be the "best possible" output, for that place and time.

For SESOIL, the approach — at the present time — would be to:

- apply simplified mathematical techniques (as described above for calibration;

- exercise the professional experience, to refine the resalts; and

- document the validation logic employed.

A schematic figure of the previously discussed processes is shown in Figure 3-13.

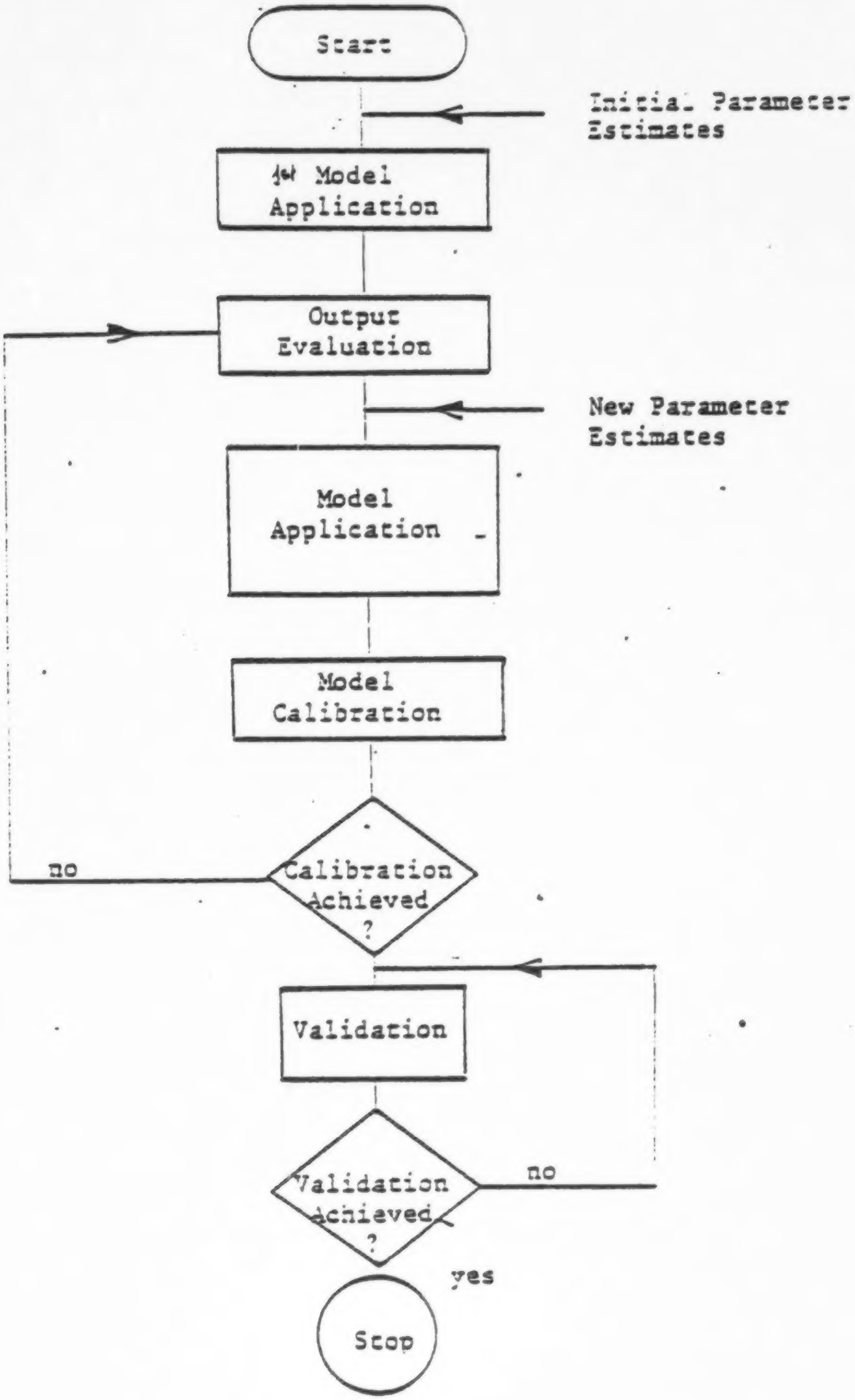

Start
Initial Parameter Estimates
1st Model Application
Output Evaluation
New Parameter Estimates
Model Application
Model Calibration
no
Calibration Achieved ?
Validation
no
Validation Achieved ?
yes
Stop

FIGURE 3-13 Schematic of Model Application, Calibration, Validation

3.4.5 Model Sensitivity Analysis

It is frequently worthwhile to perform sensitivity analyses to determine the effect on the predicted concentrations caused by a change in the input parameters. These sensitivity analyses are particularly important when data gaps or uncertain input values exist. It may also be useful to rerun SESOIL to estimate the impact of various site management or design strategies on pollutant distribution and concentrations in the environment. Two main techniques are widely used to perform sensitivity analyses:

- model simulations, and
- analytic techniques.

Model simulations are performed by running and rerunning the model while simulatneously varying the value of one or more parameters following a "scenario" logic. Model concentration predictions may be compared to monitoring data as described in the previous section.

Analytic techniques of linear systems theory (Dooge 1973) and optimization theory (Haimes 1977) may correlate sensitivity of model input (e.g., leaching quantity) to model output (e.g., soil concentrations "without" performing multiple model runs (simulations). An example is given below for an analytic technique (Fiskel et al., 1981).

Assume a SESOIL column receives pollutant input quantities $\underline{I}$ in all layers (cells). Assume as well that SESOIL employed a linear Freudlich adsorption equation, and that the average predicted adsorbed concentrations in the N cells are $\underline{c(N)}$ and that all transport is downward. Then the following matrix, linear response function $\underline{F(N)}$ can be written: -

$$\underline{I(N)} = \underline{F(N)} \cdot \underline{c(N)}$$

where F(N) is a N x N matrix:

$$\underline{F}(N) = \left| \begin{array}{ccc} & & 0 \\ f & \diagdown & \end{array} \right|$$

from which all elements N of F can be estimated. Given a possible linearity of c versus I, we can now vary input sources of the model and estimate concentration without having to run and rerun SESOIL. This approach has not been exercised by the developers; however, they may consider it in the future for certain processes and parameters.

3.4.6 Modeling Precision and Error Analysis

When applying models users are faced with issues of modeling "uncertainty," such as reliability of model prediction, and input data error propagation in model applications. Quantification of this uncertainty is of paramount importance to decision making and to optional use of fate models.

Two "uncertainties" are important in modeling the fate of pollutants in the environment. They are:

(1) The "Precision" of model predictions, in particular applications, and

(2) the "Error" characteristics of a modeling analysis.

The following two sections provide definitions for each category, and mathematical means to handle each one separately. Main emphasis is given to the "error" analysis category because, although quantitication of uncertainty has been recognized as an important aspect of fate modeling, most of the modeling exercises have focused in the "precision" question only (Donigian 1982). Thus, there exists a greater need to emphasize error analysis.

3.4.6.1 Modeling Precision

In this section, we are using "precision" not in the measurement sense (e.g., numbers of significant (digits), but to indicate those aspects of uncertainty which depend on the particular application of a model to a specific case, rather than being endemic to the model.

A precision analysis of a modeling effort can deal with questions such as: How reliable are model predictions, given a particular set of report data and a set of monitoring data; and what magnitude of error may reasonably be expected in a specific modeling exercise of future contaminant concentration given the current model of model application.

Precision analysis deals with the quantification of the "performance" or variability of a model in a given application, and is aimed at characterizing the accuracy and reliability of model results as employed to produce a specific set of field (monitoring) data. Mathematical methods used to estimate model precision have been presented by Bonazountas and Cox (1983).

3.4.6.2 Error Analysis

An error analysis deals with the question: How does an error in user input or the model itself propagate through a model, and what techniques may be employed to minimize this error.

An error analysis deals primarily with the performance of the model per se, and secondarily with the model application, and is aiming to characterize the accuracy and reliability of the model application (as contrasted to the modeling results in the precision analysis).

Traditional mathematical means to estimate propagation of an error thourh a model, have been the Monte Carlo simulation, bootstrapping, interval valued computations, nonparametric statistics, and optimization techniques. Although sound practical methods for dealing with uncertainty in environmental fate modeling are not generally available to practitioners except at the roughest level (Donigian 1983), a wealth of applicable methods are available from other branches of applied engineering (Cox 1983), including some recent work in environmental risk analysis (Cox 1983).

3.4.6.3 Mathematical Techniques

There are a variety of mathematical techniques now available for both detecting and quantifying precision, errors and uncertainties in parameter and state estimates. Methods for controlling and eliminating such uncertainties through judicious data collection are also available. (Bonazountas and Cox, 1983.)

3.4.7 Model Limitations

In general, model limitations can be due to:

- data availability,
- inoptimal single medium model application to a particular site,
- omission of important chemistry reactions, and
- lack of appropriate model validation opportunity.

Data availability refers to environmental data (e.g., climatic, soil, water resource), source data (e.g., pollutant leaching from the site), chemistry data (e.g., chemical properties of pollutants), and monitoring data (e.g., ambient concentrations). It is not appropriate, for example, to drive any soil model without a proper set of weather records and then attempt to validate the model output with available soil quality monitoring data.

Omitting certain important pathways or chemistry reactions or processes (e.g., volatilization) because of lack of data can become an issue of concern. Such pathways should be evaluated outside the model or, at certain times, by another model as far as possible. A model sensitivity analysis is essential.

3.4.8 Discussion

During the SESOIL development a number of verifications, calibration, validation and sensitivity steps have been performed to one degree or another. The model code has been verified by extensive testing under extreme conditions of input data. Each option of operation has been run multiple times and the results have been compared and rectified with sample hand calculations and by other models.

On an earlier contract to the EPA, SESOIL has been applied to two actual land treatment sites at which considerable monitoring data were available. Good agreement was obtained between monitoring data and model results. This study provided to model developer the only validation of SESOIL. These sites were also used for a sample calibration effort where the soil parameters of intrinsic permeability and adsorption coefficients were calibrated are validated to field records (Bonazountas et al., 1982).

One short study for metals has been performed (Bonazountas et al., 1982) and other short study for volatile halogenated solvents has been evaluating the overall fate of pollutants in the soil compartment, including losses to the air and to groundwater. In both studies, canonical/scenario environments were designed by combining a range of climates, soils and pollutants, in order to trace sensitivity of various parameters upon the long-term overall pollutant fate.

In the future model developers hope to extend these efforts, articularly to include increased calibrations and validations with actual field data, an essential task for model improvement and validity.

3.5 REFERENCES

Aguado, E., N. Sitar, and I Remson (1977). Sensitivity Analysis in Aquifer Studies. Journal of Geophysical Research, Vol. 13, No. 4, p. 733.

Bachmat, Y. and A. Dax (1979). An Iterative Method for Calibrating a Multicell Aquifer Model. Water Resources Research.

Bonazountas, M. and A. Cox (1983). Mathematical Error and Uncertainty Analysis in Environmental Fate Modeling. Internal Document. Arthur D. Little, Inc., Cambridge, MA 02140.

Bonazountas, M. (1983). Soil and Groundwater Fate Modeling. In: Fate of Chemicals in the Environment, Edited by R. Swann and A Eschenroeder. American Chemical Society, ACS Book Series 225, Washington, D.C.

Bonazountas, M., J. Wagner, and B. Goodwin (1982). Evaluation of Seasonal Soil/Groundwater pollutant Pathways. U.S. EPA, Data and Monitoring Support Division, EPA Contract No. 68-01-5949, Task 9, Arthur D. Little, Inc.

Brakensiek, D.L. and C.A. Onstad (1977). Parameter Estimation of the Green and Ampt Infiltration Equation. Water Resources Research, Vol. 13, No. 6, pp. 1009.

Cooley, R.L. (1977) A Method of Estimating Parameters and Assessing Reliability for Models of Steady State Groundwater Flow. 2. Application of Statistical Analysis. Water Resources, Vol. 15, No. 3, pp. 603-617.

Cox, A., H. Ojha, and F. Fiksel (1983). A Workshop on Dealing with Uncertainties in Risk Analysis. A NSF Workshop organized by Arthur D. Little, Inc., Cambridge, MA 02140.

Delhomme, J.P. (1979). Spatial Variability and Uncertainty in Groundwater Flow Parameters: A Geostatistical Approach. Water Resources Research,, Vol. 15, No. 1, pp. 269-280.

Delhomme, J.P. (1978). Driging in the Hydrosciences. Advances in Water Resources, Vol. 1, No. 5, pp. 251-266.

Dettinger, M.D. and J.L. Wilson (1981). First Order Analysis of Uncertainty in Numerical Models of Grounwater Flow. 1. Mathematical Development. Water Resources Research, Vo. 17, No. 1, pp. 149-161.

Donigian, A. (1983). Model Predictions vs. Field Observations: The Model Validization Process: Fate of Chemicals in the Environment, by R. Swann and A. Eschenroeder. ACS book series, No. 225. American Chemical Society, Washington, D.C. ISBN-0-8412-0792-5.

Donigian, A. (1982). Field Validization and Error Analysis of Chemical Fate Models. In: Dickson et al., Modeling the Fate of Chemicals in the Aquatic Environment. Ann Arbor Science, Ann Arbor, Michigan 48106, ISBM-0-250-40552-0.

Dooge, J.E. (1973). Linear Theory of Hydrologic Systems. U.S. Department of Agriculture, Washington, D.C. 20402, Technical Bulletin No. 1468.

Eagleson, P.S. (1978). Climate, Soil, and Vegetation (1-7). Water Resources Research, Vol. 14, No. 5, pp. 705-776.

Fiskel, J., M. Bonazountas, H. Ojha, and K. Scow (1981). An Integrated Geographic Approach to Developing Toxic Substance Control Strategies, Arthur D. Little, Inc., Report for the U.S. Environmental Protection Agency, Office of Policy and Resource Management. EPA Contract No. 68-01-6160.

Gambolati, G. and G. Volpi (1979). A Conceptual Deterministic Analysis of the Kriging Technique in Hydrology. Water Resources Research, Vol. 15, No. 3, pp. 625-629.

Haimes, Y.Y. (1977). Hierarchical Analyses of Water Resource Systems. McGraw Hill International Book Company, New York, ISBN 007-025507-5.

Haverkamp, R. and M. Vauclin (1979). A Note on Estimating Finite Difference Iterblock Hydraulic Conductivity Values for Transient Unsaturated Flow Problems. Water Resources Research, Vo. 15, No. 1, pp. 181.

Hayhoe, H.N. (1978). Study of the Relative Efficiency of Finite Difference and Galerkin Techniques for Modeling Soil-Water Transfer. Water Resources Research, Vol. 14, No. 1, p. 25.

McElwee, C.D. and M.A. Yukler (1978). Sensitivity of Groundwater Models with Respect to Variations in Transmissivity and Storage. Water Resources Research, Vol. 14, No. 3, pp. 451-459.

Murty, V.V.N. and V.H. Scott (1977). Determination of Transport Model Parameters in Groundwater Aquifers. Water Research, Vol. 13, No. 6, pp. 941.

Navarro, A. (1977). A Modified Optimization Method of Estimating Aquifer Parameters. Water Resources Research, Vo. 13, No. 6, pp. 935.

Nutbrown, D.A. (1975). Identification of Parameters in a Linear Equation of Groundwater Flow. Water Resources Research, Vol. 11, No.4, pp. 581.

Sagar, G, S. Yakowitz, and L. Duckstein (1975). A Direct Method for the Identification of the Parameters of Dynamic Nonhomogeneous Aquifiers. Water Resources Research, Vol. 11, No. 4, pp. 563.

Wagner, J. and M. Bonazountas (1983). Buried Halogenated Solvent Simulations vis "SESOIL." U.S. EPA, Office of Toxic Substances, EPA Contract No. 68-01-6271, Draft Report Arthur D. Little, Inc., Cambridge, MA 02140.

USER'S GUIDE TO
SESOIL EXECUTION USING THE DATA MANAGEMENT SUPPORTING SYSTEMS, SESIN AND SESOILFM

Prepared for:

U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF PESTICIDES AND TOXIC SUBSTANCES
EXPOSURE EVALUATION DIVISION
Task No. 5
Contract No. 68-02-3970
Russell Kinerson - Project Officer
Annett Nold - Task Manager

Prepared by:

GENERAL SOFTWARE CORPORATION
8401 Corporate Drive
Landover, Maryland 20785

Submitted: December 26, 1984

TABLE OF CONTENTS

PAGE NO.

I. Introduction 1

II. SESOIL Data Structure 1

- A. Input 1
- B. Output 5

III. Concept of Default Files 5

IV. Guide to SESOIL Execution and Data Management 6

- A. Access to SESOIL 6
- B. Major Decision Points in SESOIL Execution 6
- C. Detailed Guide to SESOIL Execution 7

V. Summary 11

VI. Acknowledgements 12

VII. References 12

Appendix 1. SESOIL Sample Run For 1 Year Using Both SESIN and SESOILFM 20

Appendix 2. SESOIL Sample Run For Multiple Years Using SESIN 37

Appendix 3. SESOIL Sample Run Bypassing Both SESIN and SESOILFM 50

Appendix 4. SESIN-Provided Default Files: General, Level0, Level1, Level2, and Level3 52

LIST OF TABLES AND FIGURES

Table 1. SESIN Command Summary 13
Table 2. SESOILFM Variable Summary 15
Table 3. Example of SESOILFM Product (Tabular Display) 16

Figure 1. Flowchart for SESOIL Execution with Data Management System Support 17
Figure 2. Example of SESOILFM Product (Scatter Diagram) 18
Figure 3. Example of SESOILFM Product (Cumulative Barchart) 19

I. Introduction

SESOIL is a Seasonal SOIL compartment model developed by Bonazountas and Wagner (1981) for the Office of Pesticides and Toxic Substances (OPTS) of the Environmental Protection Agency (EPA). It estimates the rate of chemical transport/transformation from the soil surface to groundwater (i.e., the unsaturated zone) in terms of mass and concentration distributions among the soil, water (i.e., the unsaturated zone) and air phases. As it was originally designed, SESOIL is batch oriented and, as such, does not support direct user interaction. The preparation and update of input data files can be manually made through the conventional text editor. The output results are in report form containing numerous parameters presented in a fixed-format fashion.

Under the auspices of the modeling team in the Exposure Evaluation Division (EED) of OPTS, the General Software Corporation (GSC) has implemented two data management systems, one for the input and one for the output, in support of the SESOIL modeling operation. The input data management system (SESIN) uses interactive prompts to assist you, the user, in the preparation of the model input files. A set of SESIN commands have been designed to perform efficient file manipulation and data editing. The output data management system (SESOILFM) provides for analyses of SESOIL output parameters, using available facilities for graphical, statistical, and tabular displays.

Additionally, a data base is available through SESIN to provide a majority of input data required by SESOIL for a total of seventy (70) cities in the United States. SESOILFM can also be used to generate an input data file for AT123D (Yeh. 1981), a transport model for the saturated zone, so that SESOIL and AT123D may be coupled to serve as a complete modeling tool for the subsurface pollutant fate analysis.

The purpose of this document is to describe in detail the procedures required to execute SESOIL through the use of the two data management systems. It is intended as a comprehensive guide for users who have no specialized computer knowledge. However, a working knowledge of the Graphical Exposure Modeling System (GEMS) (GSC 1982), through which SESOIL is executed, is necessary for making more efficient use of the SESOIL model. Only a brief description of SESOIL's input data file structure is presented to facilitate subsequent discussions. More detailed model information is contained in the original SESOIL manual (Bonazountas and Wagner 1981).

II. SESOIL DATA STRUCTURE

A. Input

Three input data files are required by SESOIL: GENERAL, LEVEL, and EXEC. Since the EXEC data file originally required by SESOIL is generated automatically by SESIN, only the GENERAL and LEVEL data files are discussed.

On the basis of the analysis need and the degree of accuracy expected in the modeling results, SESOIL allows you to select among four (4) different types (i.e., LEVEL0, LEVEL1, LEVEL2, AND LEVEL3) of LEVEL data file, each type representing a different level of data requirement sophistication. In general, the LEVEL0 and LEVEL1 data files are for analyses on an annual basis (one year only) of a 2-layer soil column. The LEVEL2 data file is for analyses on a monthly basis (from 1 through 10 years) of a 2-layer soil column. The LEVEL3 data file is similar to the LEVEL2 data file with the exception that the soil column is sliced into a 3-layer configuration. A detailed presentation of these data files is given below.

1. GENERAL DATA FILE

This data file contains the following climatologic, soil, and chemical input parameters:

-- Climatologic

L	Latitude of area (degree N)
TA	Temperature of area (degree C)
NN	Fraction of area covered by clouds (fraction)
S	Relative humidity of area (fraction)
A	Shortwave albedo of surface (-)
REP	Daily evaportranspiration (cm/day)
MPA	Annual precipitation (cm)
MPM	Monthly precipitation (cm)
MTR	Mean time of rain (days)
MN	Mean number of storm events (#)
MT	Mean length of rainy season (days)

(Note: All parameters are presented either yearly or monthly, depending on the selected type of the LEVEL data file. MPA is used for LEVEL0 and LEVEL1 only)

-- Soil

RS	Soil density (g/cm^3)
K1	Soil intrinsic permeability (cm^2)
C	Soil disconnectedness index (-)
N	Effective soil porosity (-)
OC	Organic content of soil (% OC)
CC	Clay content of soil (% CC)
CEC	Soil cation exchange capacity (me/100g)
K1U	Intrinsic permeability of upper soil layer (cm^2)

K1M	Intrinsic permeability of middle soil layer (cm^2)
K1L	Intrinsic permeability of lower soil layer (cm^2)

(Note: All the above parameters are not necessarily needed for a given type of LEVEL data file.)

-- Chemical

SL	Compound solubility in water (ug/ml)
KOC	Adsorption coeff in organic carbon (ug/goc)/(ug/ml)
DA	Diffusion coeff in air (cm^2/sec)
KDE	Biodegradation rate of compound (day^{-1})
H	Henry's law constant (m^3*atm/degK*mol)
K	Adsorption coeff in soil (ug/g)/(ug/m)
MWT	Molecular weight (g/mol)
VAL	Valence
KNH	Neutral hydrolysis constant (day^{-1})
KBH	Base hydrolysis constant (L/mol*day)
KAH	Acid hydrolysis constant (L/mol*day)
SK	Stability constant compound-lig and complex(-)
B	Moles of lig and per mole of compound complexed [#]
MWTLIG	Molecular weight of lig and (g/mol)

2. LEVELO Data File

This data file contains the following input parameters:

AR	Surface area of the compartment (cm^2)
Z	Depth to groundwater table (m)
DU	Depth of upper soil zone (cm)
PH	pH of upper soil zone (-)
APH	Ratio: pH lower to upper soil zone (-)
AKDE	Ratio: biodegradation rate lower to upper soil zone (-)
AOC	Ratio: Organic carbon lower to upper soil zone (-)
ACC	Ratio: Clay content lower to upper soil zone (-)
ISRA	Index of surface runoff participation in pollutant transport (-)
ASL	Ratio: Pollutant conc. in rain to maximum solubility in water (-)
ACEC	Ratio: CEC lower to upper soil zone (-)
POLINU	Total pollutant load per year entering upper soil zone (ug/cm^2)

POLINL	Total pollutant load per year entering lower soil zone (ug/cm^2)
LIGU	Lig and input mass to upper soil zone (ug/cm^2)
LIGL	Lig and input mass to lower soil zone (ug/cm^2)
THA	Soil moisture content (%)
IA	Infiltration (cm)
RGA	Groundwater recharge (cm)
RSA	Surface runoff (cm)

3. LEVEL1 Data File

This data file contains all the input parameters listed for the LEVELO data file except THA, IA, RGA, and RSA.

4. LEVEL2 Data File

This data file contains the following input parameters:

AR	Surface area of the compartment (cm^2)
Z	Depth to groundwater table (m)
DU	Depth of upper soil zone (cm)
PH	pH of upper soil zone (-)
APH	Ratio: pH lower to upper soil zone (-)
AKDE	Ratio: biodegradation rate lower to upper soil zone (-)
AOC	Ratio: Organic carbon lower to upper soil zone (-)
ACC	Ratio: Clay content lower to upper soil zone (-)
FRN	Freundlich equation exponent (-)
ACEC	Ratio: CEC lower to upper soil zone (-)
CUM	Conc. pollutant in soil moisture upper zone (g/ml)
CLM	Conc. pollutant in soil moisture lower zone (g/ml)
POLINU	Pollutant load per unit area entering upper zone (ug/cm^2)
POLINL	Pollutant load per unit area entering lower zone (ug/cm^2)
ISRM	Monthly index for pollutant appearance in surface runoff (-)
ASL	Monthly ratio: conc. of pollutant to maximum solubility in H_2O (-)
TRANSU	Pollutant transformed in upper zone (ug/cm^2)
TRANSL	Pollutant transformed in lower zone (ug/cm^2)
SINKU	Pollutant lost by processes not described (upper) (ug/cm^2)

SINSL	Pollutant lost by processes not described (lower) (ug/cm^2)
LIGU	Lig and mass input to upper zone (ug/cm^2)
LIGL	Lig and mass input to lower zone (ug/cm^2)

(Note: Parameters CUM through LIGL are expressed in terms of monthly values)

5. LEVEL3 Data File

This data file is, in structure, almost identical to LEVEL2 data file with the exception of additional entries for the third (middle) soil layer.

Examples of the GENERAL, LEVEL0, LEVEL1, LEVEL2, and LEVEL3 data files are given in Appendix 3. Note that:

- The GENERAL data file contains data for different sites, soil types, and chemical compounds.
- For simulation period of more than one year (LEVEL2 or LEVEL3 application), the input parameters can be repeated for each additional year under consideration for up to 10 years.
- For simulation of many years of data (up to 100 years) for a desired scenario of pollutant loadings, an auxiliary file (AUX) can be created which contains the variables POLINU, POLINL (LEVEL2) and POLINM (LEVEL3). The user is prompted to build this file only if the number of years of available data in the GENERAL and LEVEL files are less than the desired number of years to be simulated as given by the parameter JYRS in the EXEC data file.
- LEVEL0, LEVEL1, and LEVEL2 data files also contain data for more than one site location.

B. Output

Output results of SESOIL include hydrologic balance calculations and the distribution of pollutant in the soil column. After successfully following the procedures described in this document, you are able to obtain a complete hard-copy SESOIL output for review. A total of 86 selected SESOIL output parameters can be stored in GEMS for further analysis.

III. CONCEPT OF DEFAULT FILES

To minimize the complications involved in the preparation of SESOIL input data files, the design of SESIN is based on the central concept of providing you with a complete set of default files with which you can perform all necessary file editing and manipulations. In requesting the default files, there are three options supported by SESIN:

1. The default files are retrieved from the 70-city data base (Note: This data base only provides data for Level 3 operation).

2. The default files are retrieved from the files presented in Appendix 3.

3. The default files are specified by you.

The use of Option 1 is illustrated in Appendix 1. Note that once these default files are available to you, you must review all the default values carefully to check their applicability to your simulation run. In some cases, some default values are provided for you only to ensure the completeness of the file content and they must be revised by you in order to give meaningful simulation results.

IV. GUIDE TO SESOIL EXECUTION AND DATA MANAGEMENT

A. Access to SESOIL

You can access SESOIL through the Graphical Exposure Modeling System (GEMS). The host computer of GEMS is Digital Equipment Corporation VAX-11/780, located at EPA's National Computer Center (NCC) in Research Triangle Park, North Carolina.

It is assumed that you are familiar with the log-on procedures of the VAX system and are able to invoke GEMS (Consult User's Guide to GEMS, if not). After you make connection, the two steps required to gain access to SESOIL in GEMS are:

```
ENTER AN OPERATION:   M    <CR>

ENTER MODEL NAME:     SESOIL <CR>
```

* (Where <CR> stands for pressing the carriage return key on the terminal).

B. Major Decision Points in SESOIL Execution

At the outset, and through the process of SESOIL execution, you are confronted with the following major decision points:

(1) Do I have all the GENERAL, LEVEL (LEVEL0, LEVEL1, LEVEL2, or LEVEL3), EXEC, and AUX (if necessary) data files ready for execution , so that I do not need to create those data files through SESIN? (Note: (a) The EXEC data file is required if SESIN is not used. Refer to the original SESOIL manual for description. (b) The AUX file is required if JYRS in the EXEC data file is greater than the number of years of data available in the LEVEL and GENERAL data files.)

(2) If I use SESIN support, which of the three options (see Section III) do I choose to get my default GENERAL and LEVEL data files?

(3) Do I want to generate additional years of pollutant loading data?

(4) Do I want to make multiple SESOIL runs?

(5) Do I want the support of the output data management system, SESOILFM, so that after the SESOIL execution is completed, I can perform graphical, statistical, and tabular output manipulations using GEMS' facilities?

(6) If the answer to (5) is "yes", what is the dataset name (1 to 12 characters) under which I want my SESOIL output to be stored in GEMS?

(7) Do I want to request an AT123D input file based on the SESOIL simulation results?

(8) If the answer to (7) is "yes", do I want to make an AT123D run using the AT123D input file just created?

A flowchart outlining the relative sequence of the above decision points is presented in Figure 1. As shown, the entire process can be divided into five execution branches which will be discussed below.

C. Detailed Guide to SESOIL Execution

To facilitate the following discussion, this section will be presented in terms of the five execution branches shown in Figure 1.

1. Branch 1

This is the core of the GSC-developed SESOIL data management system. The execution will enter this branch if you choose to create new data files (i.e. GENERAL and LEVEL data files) through SESIN. The main idea is to guide you interactively through an efficient data editing and file preparation process. To do this, SESIN is equipped with the following user commands:

```
ALL     BRIEF    <CR>     DONE    EXIT      HELP
LA120   LAST     MENU     NEXT    NOBRIEF   NONE
REST    REVIEW   REVISE   VT100
```

A detailed list of command descriptions is presented in Table 1. cities

To start with, you need to select one of the three options for getting you default data files (see Section III). After the selection, you are guided by self-explanatory prompts provided by SESIN. You can respond with brief answers or use the above listed commands to control the progress of the process. The use of SESIN and its commands can be illustrated best by Appendix 1, which contains a step-by-step example side-marked with comments. You are advised to follow this example carefully in order to make efficient use of SESIN. It is to be stressed that Appendix 1 only presents an entry-level demonstration of the use of SESIN. After becoming more familiar with the organization of SESOIL input files and the concepts of SESIN, you are encouraged to explore the other powerful SESIN capabilities through hands-on trail practices.

1.a. Branch 1-A

This branch is a sub branch of Branch 1. It represents the use of generating long-term pollutant application scenarios. The execution will enter this branch if the value of JYRS (desired number of years to be simulated) in the EXEC data file (as specified by the user) is greater than the number of years of data available in the GENERAL and LEVEL data files. If this is true, the user is prompted to specify the additional pollutant loading data (POLINU, POLINM, POLINL) for the additional years required, which is then stored in the auxiliary data file AUX. The remaining parameter values of the GENERAL and LEVEL data files for the additional years are automatically generated by repeated use of the last year of data. An example run using this Branch is given in Appendix 2.

2. BRANCH 2

This branch represents the original SESOIL data file input fashion in that it prompts you to input directly the three data files: GENERAL, LEVEL (i.e., LEVEL0, LEVEL1, LEVEL2, or LEVEL3), and EXEC. The auxiliary pollutant loading data file, AUX is also prompted for. Note that the user-prepared EXEC data file is needed in this branch. The SESOIL execution will enter this branch if you select not to create new data files through SESIN. An example is given in Appendix 3 to illustrate the use of this branch.

3. BRANCH 3

This branch represents the use of the GSC-developed SESOIL output data management system (SESOILFM), which allows you to create a dataset containing 86 selected SESOIL output variables, as shown in Table 2. This dataset will be stored in GEMS so that you can utilize GEMS' capabilities for output data manipulation, analysis, and interpretation. The columns of VAR NAME and VAR UNIT in Table 2 give brief variable definitions and variable units, respectively, to assist you in recognizing the variables to be selected for further review. Note that Variables 5 through 7, representing chemical half-life periods for different soil layers are not direct SESOIL output variables. Instead, they are derived from the degradation rates (Variables 2 through 4) of chemicals assuming a first order decay. Furthermore, Variables 73 through 86, each representing a possible transformation/transport process in the pollutant fate analysis, are calculated from the SESOIL output to show the total mass balance distribution in the unstaurated soil zone at the end of each year being simulated. Each of the variables in Table 2 is stored in the dataset on a monthly basis (i.e., not monthly applicable, such as PRECIP, MASGRW, etc.), their estimated values are stored in the dataset at the 12th month of each year. Spaces prior to the 12th month are flagged as "NO VALUE".

In addition to the variables shown in Table 2, the following identification and time-factor variables are included in the dataset to facilitate the use of GEMS' capabilities.

RUN:	Run identification number
COMP ID:	Compound name studied
LEVEL:	Modeling level selected
YEAR:	Year simulated
MONTH:	Cumulative month through the years simulated
MINDEX:	Month of given year (non-cumulative)
VAR ID:	Variable identification code (to be used to call out the variable needed)
VAR NAME:	More descriptive variable definition
VAR UNIT:	Unit for each variable

As shown, each of these variables serves a specific identification purpose. You can also use the variable RUN to retrieve (via GEMS EXTRACT and/or FILTER function) the variables for a particular run from a dataset containing multiple run records. The variable MONTH provides an across-the-years monthly time index, which you can use to observe the continuous variation of a given variable throughout the years being analyzed.

There are only three steps required to use SESOILFM for creating a SESOIL output dataset in GEMS, as exemplified near the end of Appendix 1. The steps are:

(i) enter Y in response to the prompt: "Enter Y to output SESOIL results to GEMS>"

(ii) give a dataset name (1 to 12 characters) in response to the prompt: "Enter GEMS output dataset name>"

(iii) enter a dataset description (1 to 60 characters) in response to the prompt: "Enter tag field>."

Any characters other than Y entered in Step (i) cause the execution to skip the the SESOILFM supporting service. The tag field is optional and you use it only for the purpose of more descriptive dataset identification. You can skip this entry by pressing <CR>.

It is beyond the scope of this document to describe the applications of GEMS' graphical, statistical, and tabular facilities to the SESOIL dataset described above. You are advised to consult the User's Guide to GEMS (GSC 1982) for detailed information. However, to demonstrate what kind of products you may obtain from the use of SESOILFM and GEMS file management facilities, the following examples are presented:

Figure 2: This is a display of the predicted monthly pollutant mass transport into the groundwater (INMOGRW) vs. the cummulative month index (MONTH) for a period of four years. The two curves, presenting a vivid visual comparison, are derived from two separate SESOIL runs, one with a biodegradation rate (KDE) of 1.0 day $^{-2}$ and the other of 0.22 day $^{-2}$.

Figure 3: This is a bar chart showing the cumulative effect of the curve with a KDE of 1.0 day $^{-2}$ in Figure 2.

Table 3: This is a GEMS' tabular output presenting the four variables: MONTH, MINDEX, CONWMOU, MASWMOU. Note that Table 2 is also produced using SESOILFM and GEMS.

4. BRANCH 4

This branch is activated if you elect to bypass SESOILFM by entering any characters other than Y in response to the prompt: "Enter Y to output SESOIL results to GEMS>". An example of this is shown near the end of Appendix 1.

5. BRANCH 5

This branch allows you to review the SESOIL results that are applicable to the construction of an AT123D input file. After review, if you are satisfied with the results, you can request the build up of an AT123D input file. Due to the complexity of the file content, the following assumptions are used:

- The pollutant source area is assumed to be a square with a size equivalent to the soil column area used in SESOIL.
- The aquifer depth and width are assumed to be infinite.
- The hydraulic gradient is assumed to be 0.01.
- The hydraulic conductivity is based on SESOIL's intrinsic permeability.
- The longitudinal, transverse, and vertical dispersivities are assigned on the basis of Yeh's (1981) typical values and the calculated hydraulic conductivity.
- The time interval size is assumed to be 8760 hours (i.e., one year for level 2 and 3; 730 hours (i.e., one month) for level 0 and 1.

- The loading source release is assumed to be constant (NSOUS=0) for level 0 and 1; time-dependent (NSOUS=0) for level 2 and 3.
- The loading source release is assumed to be instantaneous (INSTAN=0) for level 0 and 1; continuous (INSTAN=1) for level 2 and 3.
- The time duration of waste release is assumed to continue through the entire SESOIL simulation period for level 2 and 3; not used for level 0 and 1.
- The variable source release rate, calculated by SESOIL, is used for level 2 and 3.
- The decay constant is set equivalent to the neutral hydrolysis rate used in SESOIL.
- The distribution coefficient is taken as equal to the adsorption coefficient used in SESOIL.

Several of the assumptions which may require special attention are printed as "Notes" in the Branch-5 output as shown in the sample run in Appendix 1.

In addition to the above assumptions, the AT123D input file is also developed using various assumed program functional and execution control values. You must carefully review the file content to ensure the applicability of all input values to your specific need. You can edit or execute this AT123D input file using the AT123D data management systems, AT123DIN and AT123DOUT, by responding to the last prompt in Appendix 1 with a "yes". For more information concerning the use of AT123D data management systems, consult the AT123D User's Guide (GSC, 1983).

V. SUMMARY

A concise guide to SESOIL execution using GSC-developed input (SESIN) and output (SESOILFM) data management systems is presented in this document. The basic SESOIL data structure is discussed briefly to provide the necessary background for the efficient use of SESIN and SESOILFM. The execution logic is outlined by five major branches, each of which may be invoked or bypassed by you using interactive commands. Most importantly, detailed examples (Appendix 1 and Appendix 2) with step-by-step explanatory comments are provided to guide the user through a successful test SESOIL execution. The user is advised to follow those examples closely to ensure the most efficient use of the systems.

Again, it is to be stressed that Appendices 1, 2 and 3 present only an entry-level demonstration of the use of SESIN and SESOILFM, respectively. The more advanced capabilities of these two systems can be learned via hands-on trial practices. For assistance, call GSC at (301) 459-9494.

VI. ACKNOWLEDGEMENTS

The development of the SESOIL execution supporting systems, SESIN and SESOILFM, was sponsored by the Office of Pesticides and Toxic Substances of the U.S. Environmental Protection Agency. Helpful comments were received from Dr. Annett Nold and Dr. Russell Kinerson.

The following general Software Corporation staff participated in the SESIN and SESOILFM development:

Project Manager: Jon Chen

Program Design and Coordination: James Pilotte, Yann King, Stuart Wollman

SESIN Programming: Dalroy Ward

SESOILFM Programming: Judy Chen

VII. REFERENCES

Bonazountas M, Wagner JM. 1981. A seasonal soil compartment model. Arthur D. Little, Inc. Draft report.

General Software Corp. 1982. User's guide to the Graphical Exposure Modeling System (GEMS). Draft report. Washington, D.C.: Office of Pesticides and Toxic Substances, U.S. Environmental Protection Agency. Contract 68016618

General Software Corp. 1984. User's guide to AT123D execution using the data management supporting system, AT123DIN and AT123DOUT. Draft report.

Yeh, G.T. 1981. "AT123D: Analytical Transient One-, Two-, and Three-Dimensional Simulation of Waste Transport in the Aquifer System", ORNL-5602. Oak Ridge National Laboratory, Oak Ridge, TN.

TABLE 1. SESIN COMMAND SUMMARY

```
 The following is a list of commands that apply within SESIN.  Note that
all commands do not work at all prompts.

ALL       BRIEF     <CR>      DONE      EXIT      HELP      LA120
LAST      MENU      NEXT      NOBRIEF   NONE      REST      REVIEW
REVISE    VT100

for additional help with a command type: HELP <COMMAND>
for a full list of commands with explainations type: HELP *

ALL             - for parameter input ALL designates that all
                  parameters will be changed.
                - in response to a request for a list of months
                  ALL designates that values for all 12 months
                  will be set to a single input value.

BRIEF           - no parameter descriptions will be given when a parameter
                  menu is displayed.

<CR>            - a carriage return assumes the currently selected
                  data.

DONE            - previous input and existing values are accepted
                  and program execution continues with the next
                  prompt.

EXIT            - the program run is immediately ended if no runs have
                  yet been fully set up.  If at least one run has been
                  set up you will go through the exit procedure which
                  will create your run files.  If you type exit again
                  at this point the program run will be immediately stoped.

HELP            - provides command summary and descriptions.

LA120           - informs the program that the user is on an LA120
                  or other hardcopy terminal. Program output is
                  slightly modified for this terminal type.  This
                  is the default terminal type.

LAST            - this command can be used to modify climatic or
                  level data for the year preceeding the current
                  year.  This is particularly useful when using
                  the revise command to modify data from a prior
                  run.
```

TABLE 1. SESIN COMMAND SUMMARY(CONTINUED)

MENU	- displays the current parameter list when at a data item prompt.
NEXT	- this command is the complement to the LAST command and can be used to move forward a year in a climatic or level data set.
NOBRIEF	- allows display of parameter descriptions to be restored after BRIEF has been used.
NONE	- at site,chemical,or soil selection this command allows the zeroing of the input data array for entry of an entirely new set of data. - at all other prompts NONE is identical to DONE
REST	- allows the user to copy the remainder of the default input data file to the sesoil input file being developed. This command only works at the enter data item to be updated prompt for monthly level or climatic data.
REVIEW	- allows the user to review the current data set. The user is prompted to enter C or A for review to review either data for just the current year or for all years up to the current year.
REVISE	- allows modification of the currently selected data (level, climatic, soil or chemical). This command is used when making multiple runs which require modification of data selected in the previous run. - NOTE when this command is used when in level 2 or 3 (monthly data) you will be left at the last data year entered when altering monthly parameters.
VT100	- this command turns off the LA120 command and can be used for all CRT terminals.

TABLE 2. SESOILFM VARIABLES SUMMARY

#	VAR ID	VAR NAME	VAR UNIT
1	DEPTHGRW	DEPTH TO GRW	METER
2	DEGRDU	DEGRAD. RATE(U)	PER DAY
3	DEGRDM	DEGRAD. RATE(M)	PER DAY
4	DEGRDL	DEGRAD. RATE(L)	PER DAY
5	HALFU	HALF-LIFE(U)	MONTH
6	HALFM	HALF-LIFE(M)	MONTH
7	HALFL	HALF-LIFE(L)	MONTH
8	ADSOIL	ADSORP CO(SOIL)	(UG/G)/(UG/ML)
9	ADOC	ADSORP CO(O.C.)	(UG/GOC)/(UG/ML
10	%OCU	% ORG. CARB.(U)	%
11	%OCM	% ORG. CARB.(M)	%
12	%OCL	% ORG. CARB.(L)	%
13	HENRY	HENRY CONSTANT	CU M-ATM/MOLE
14	DENSITY	SOIL DENSITY	G/CU M
15	PERMALL	INTRA PERM(AVE)	SQ CM
16	PERMU	INTRA PERM(U)	SQ CM
17	PERMM	INTRA PERM(M)	SQ CM
18	PERML	INTRA PERM(L)	SQ CM
19	POROSITY	SOIL POROSITY	---
20	PRECIP	YEARLY PRECIP.	CM
21	INYRU	POL YR INPUT(U)	UG
22	INMOU	POL MO INPUT(U)	UG/SQ CM
23	INYRM	POL YR INPUT(M)	UG
24	INMOM	POL MO INPUT(M)	UG/SQ CM
25	INYRL	POL YR INPUT(L)	UG
26	INMOL	POL MO INPUT(L)	UG/SQ CM
27	MOIST	SOIL MOISTURE	%
28	GRWFLOW	GRW RUNOFF	CM
29	DEGRYRU	YR DEGRADED(U)	UG
30	DEGRMOU	MO DEGRADED(U)	UG
31	DEGRYRM	YR DEGRADED(M)	UG
32	DEGRMOM	MO DEGRADED(M)	UG
33	DEGRYRL	YR DEGRADED(L)	UG
34	DEGRMOL	MO DEGRADED(L)	UG
35	INYRGRW	YR INTO GRW	UG
36	INMOGRW	MO INTO GRW	UG
37	CONWYRU	YR CONC-MOIS(U)	UG/ML
38	CONWYRM	YR CONC-MOIS(M)	UG/ML
39	CONWYRL	YR CONC-MOIS(L)	UG/ML
40	CONWMOU	MO CONC-MOIS(U)	UG/ML
41	CONWMOM	MO CONC-MOIS(M)	UG/ML
42	CONWMOL	MO CONC-MOIS(L)	UG/ML
43	CONSYRU	YR CONC-SOIL(U)	UG/G
44	CONSYRM	YR CONC-SOIL(M)	UG/G
45	CONSYRL	YR CON-SOIL(L)	UG/G
46	CONSMOU	MO CONC-SOIL(U)	UG/G
47	CONSMOM	MO CONC-SOIL(M)	UG/G
48	CONSMOL	MO CONC-SOIL(L)	UG/G
49	MASWYRU	YR MASS-MOIS(U)	UG
50	MASWYRM	YR MASS-MOIS(M)	UG
51	MASWYRL	YR MASS-MOIS(L)	UG
52	MASWMOU	MO MASS-MOIS(U)	UG
53	MASWMOM	MO MASS-MOIS(M)	UG
54	MASWMOL	MO MASS-MOIS(L)	UG
55	MASSYRU	YR MASS-SOIL(U)	UG
56	MASSYRM	YR MASS-SOIL(M)	UG
57	MASSYRL	YR MASS-SOIL(L)	UG
58	MASSMOU	MO MASS-SOIL(U)	UG
59	MASSMOM	MO MASS-SOIL(M)	UG
60	MASSMOL	MO MASS-SOIL(L)	UG
61	CONAYRU	YR CONC-AIR(U)	UG/ML
62	CONAYRM	YR CONC-AIR(M)	UG/ML
63	CONAYRL	YR CONC-AIR(L)	UG/ML
64	CONAMOU	MO CONC-AIR(U)	UG/ML
65	CONAMOM	MO CONC-AIR(M)	UG/ML
66	CONAMOL	MO CONC-AIR(L)	UG/ML
67	MASAYRU	YR MASS-AIR(U)	UG
68	MASAYRM	YR MASS-AIR(M)	UG
69	MASAYRL	YR MASS-AIR(L)	UG
70	MASAMOU	MO MASS-AIR(U)	UG
71	MASAMOM	MO MASS-AIR(M)	UG
72	MASAMOL	MO MASS-AIR(L)	UG
73	MASSURF	MASS IN SURF	%
74	MASGRW	MASS IN GRW	%
75	MASVOLA	MASS VOLATILIZE	%
76	MASSINK	MASS IN SINKS	%
77	MASSOIL	MASS ON SOIL	%
78	MASCECIM	MASS IMMOBILIZE	%
79	MASDEGRD	MASS DEGRADED	%
80	MASHYMOI	MASS HYDRO.-MOI	%
81	MASHYSOI	MASS HYDRO.-SOI	%
82	MASHYCEC	MASS HYDRO.-CEC	%
83	MASCCMPL	MASS COMPLEXED	%
84	MASTRANS	MASS TRANSFORME	%
85	MASMOI	MASS IN MOIST.	%
86	MASAIR	MASS IN AIR	%

U: UPPER SOIL LAYER

M: MIDDLE SOIL LAYER

L: LOWER SOIL LAYER

YR: YEARLY

MO: MONTHLY

TABLE 3. EXAMPLE OF SESOILFM PRODUCT(TABULAR DISPLAY)

```
#    | MONTH              | MINDEX            | CONWMOU           | MASWMOU          |
---------------------------------------------------------------------------------------
   1 |                  1 |                 1 | 0.37293001E-02 |    86906.555     |
   2 |                  2 |                 2 | 0.74580982E-02 |    173801.42     |
   3 |                  3 |                 3 | 0.11186397E-01 |    260684.66     |
   4 |                  4 |                 4 | 0.14914199E-01 |    347556.31     |
   5 |                  5 |                 5 | 0.18641606E-01 |    434418.75     |
   6 |                  6 |                 6 | 0.22368507E-01 |    521269.41     |
   7 |                  7 |                 7 | 0.26095007E-01 |    608110.75     |
   8 |                  8 |                 8 | 0.29821001E-01 |    694940.19     |
   9 |                  9 |                 9 | 0.33546392E-01 |    781755.69     |
  10 |                 10 |                10 | 0.37271384E-01 |    868561.88     |
  11 |                 11 |                11 | 0.40995900E-01 |    955356.94     |
  12 |                 12 |                12 | 0.44719987E-01 |    1042142.0     |
  13 |                 13 |                 1 | 0.48443485E-01 |    1128913.4     |
  14 |                 14 |                 2 | 0.52166484E-01 |    1215673.1     |
  15 |                 15 |                 3 | 0.55889081E-01 |    1302423.4     |
  16 |                 16 |                 4 | 0.59611194E-01 |    1389162.5     |
  17 |                 17 |                 5 | 0.63332774E-01 |    1475889.1     |
  18 |                 18 |                 6 | 0.67053966E-01 |    1562606.8     |
  19 |                 19 |                 7 | 0.70774674E-01 |    1649313.1     |
  20 |                 20 |                 8 | 0.74494869E-01 |    1736007.4     |
  21 |                 21 |                 9 | 0.78214593E-01 |    1822690.9     |
  22 |                 22 |                10 | 0.81933878E-01 |    1909364.1     |
  23 |                 23 |                11 | 0.85652687E-01 |    1996026.1     |
  24 |                 24 |                12 | 0.89371011E-01 |    2082676.9     |
  25 |                 25 |                 1 | 0.93088754E-01 |    2169314.0     |
  26 |                 26 |                 2 | 0.96806012E-01 |    2255940.0     |
  27 |                 27 |                 3 | 0.10052200     |    2342536.5     |
  28 |                 28 |                 4 | 0.10423800     |    2429133.0     |
  29 |                 29 |                 5 | 0.10795202     |    2515683.5     |
  30 |                 30 |                 6 | 0.11166400     |    2602186.5     |
  31 |                 31 |                 7 | 0.11537600     |    2688689.8     |
  32 |                 32 |                 8 | 0.11908799     |    2775193.3     |
  33 |                 33 |                 9 | 0.12280001     |    2861697.0     |
  34 |                 34 |                10 | 0.12651201     |    2948200.3     |
  35 |                 35 |                11 | 0.13022399     |    3034703.3     |
  36 |                 36 |                12 | 0.13393600     |    3121207.0     |
```

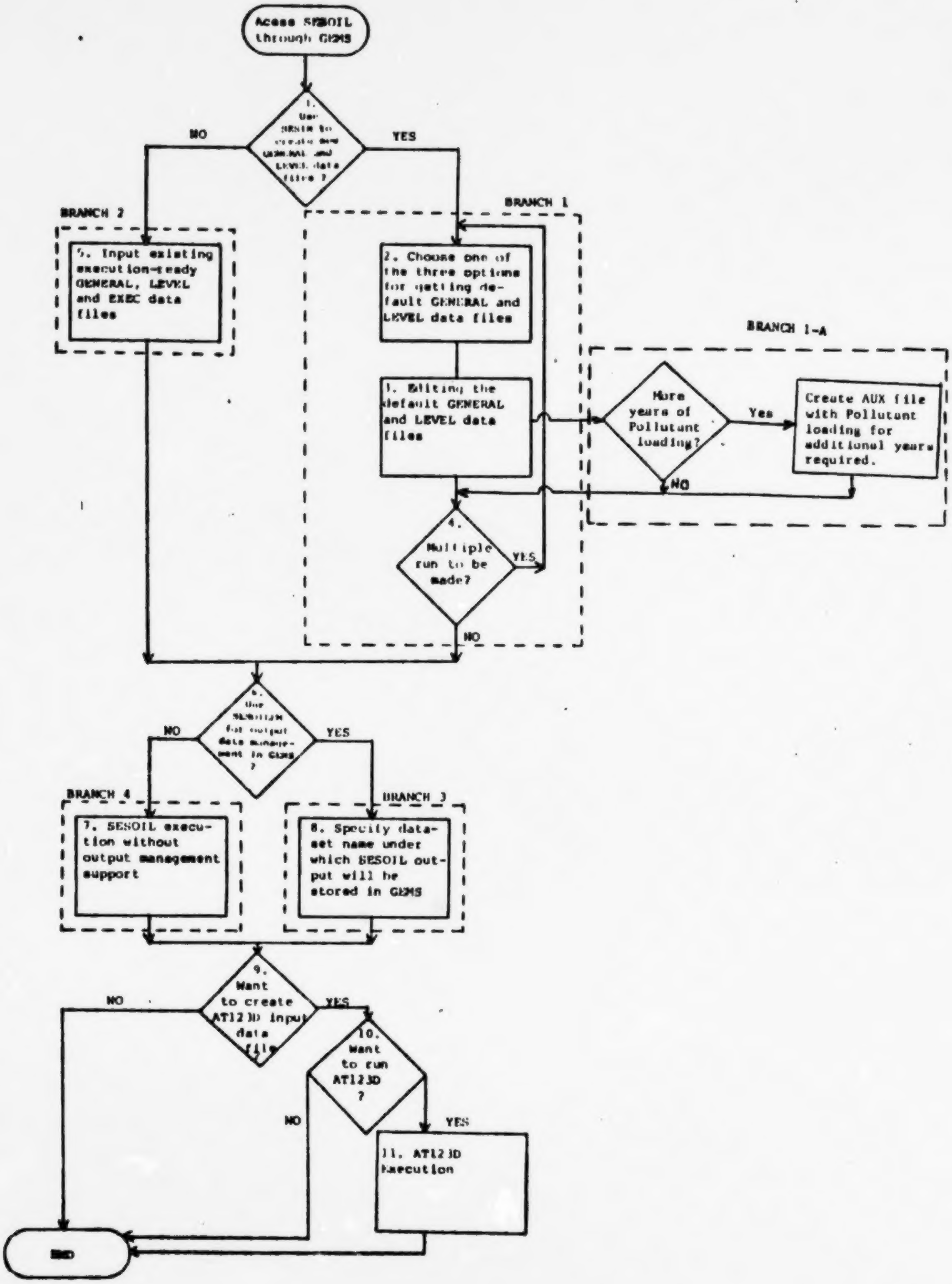

Access SESOIL through GEMS
1. Use create new GENERAL and LEVEL data files ?
NO
YES
BRANCH 2
5. Input existing execution-ready GENERAL, LEVEL and EXEC data files
BRANCH 1
2. Choose one of the three options for getting default GENERAL and LEVEL data files
3. Editing the default GENERAL and LEVEL data files
BRANCH 1-A
More years of Pollutant loading?
Yes
Create AUX file with Pollutant loading for additional years required.
NO
4. Multiple run to be made?
YES
NO
6. Use for output data management in GEMS ?
NO
YES
BRANCH 4
7. SESOIL execution without output management support
BRANCH 3
8. Specify dataset name under which SESOIL output will be stored in GEMS
9. Want to create AT123D input data file
NO
YES
10. Want to run AT123D ?
NO
YES
11. AT123D Execution
END

FIGURE 1. FLOWCHART FOR SESOIL EXECUTION WITH DATA MANAGEMENT SYSTEM SUPPORT

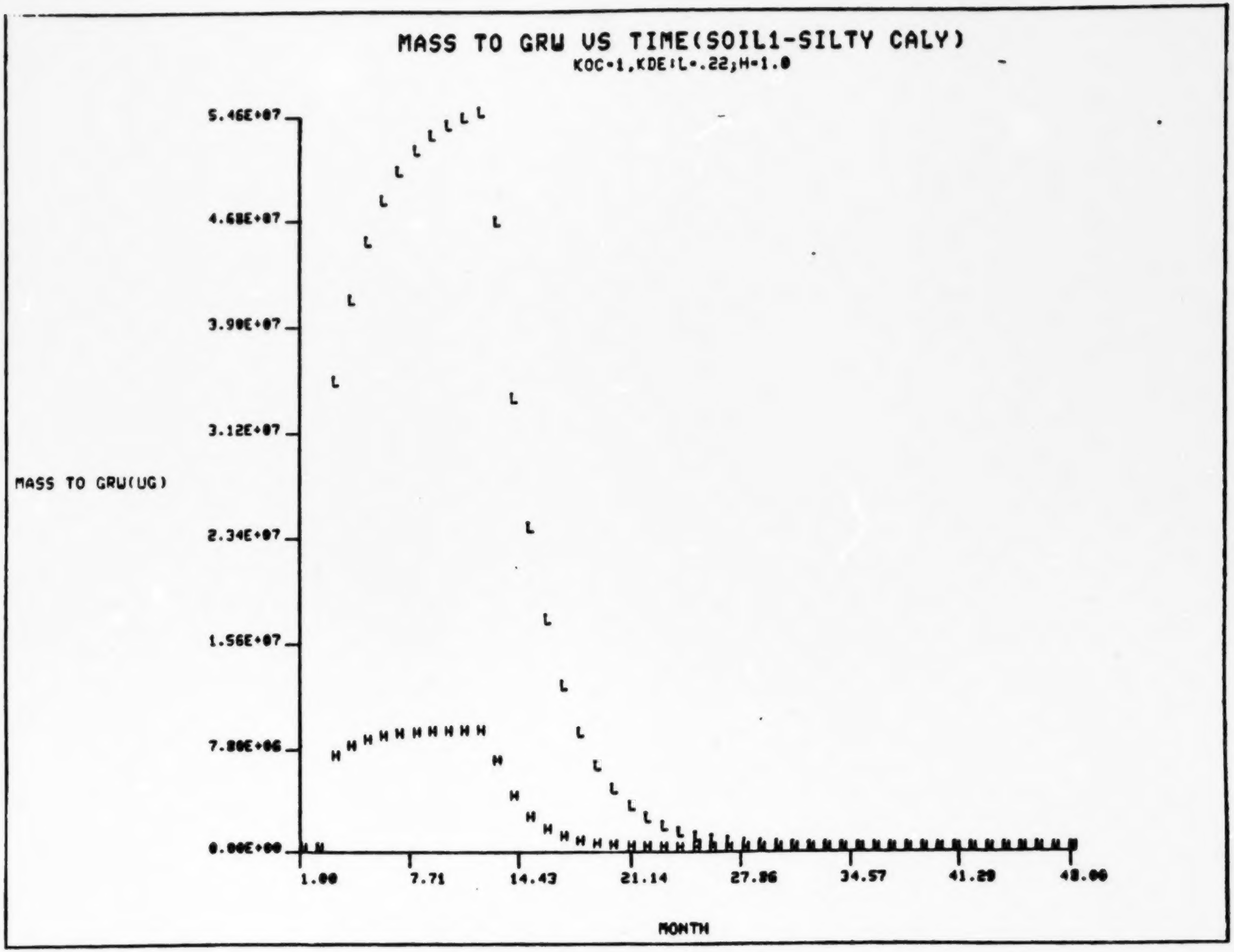


FIGURE 2. EXAMPLE OF SESOILFM PRODUCT(SCATTER DIAGRAM)

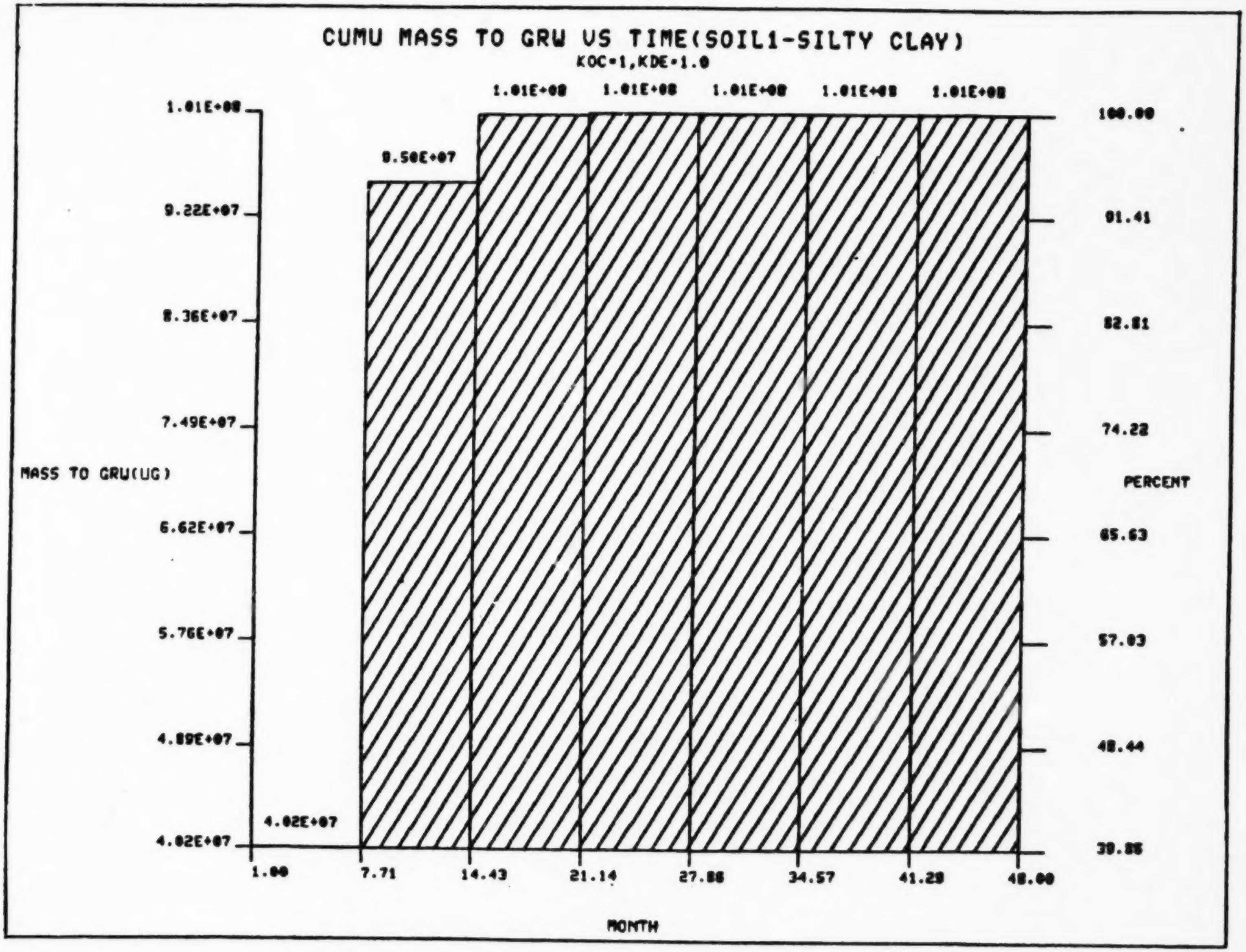


FIGURE 3. EXAMPLE OF SESOILFM PRODUCT(CUMULATIVE BARCHART)

APPENDIX 1: SESOIL SAMPLE RUN FOR 1 YEAR USING BOTH SESIN AND SESOILFM

```
Enter an operation: [m]

Enter a model name: [sesoil]

                                    NOTE
                        *******************************
                        These are the two steps required
                        to access SESOIL through GEMS.
                        [ ] encloses your response.


Are you creating SESOIL input files: [yes]

                                    NOTE
                        *******************************
                        This is the decision to enter
                        either BRANCH 1 or BRANCH 2
                        (see figure 1).


                                         SESIN
                                 INTERACTIVE SESOIL INPUT
                                       GSC VER1.1
                                        5-DEC-84

For a list of commands type : HELP COMMANDS


Do you want to use data from the cities database? [yes]

Enter the name of the desired data site: [help]

                                    NOTE
                        *******************************
                        'help' was used to get
                        assistance from the system.


A PLACE NAME            THE NAME OF A DATA SITE IN THE DATABASE
LIST                    TO LIST ALL THE AVAILABLE DATA SITES
EXIT                    TO EXIT THE PROGRAM
HELP                    TO OBTAIN THESE MESSAGES

Enter the name of the desired data site: [list]

                                    NOTE
                        *******************************
                        Based on the help information,
                        'list' was used to show all the
                        sites in the cities database.
```

```
Enter the state abbreviation or ALL for entire list [all]

                              NOTE
                 ******************************
                 A list containing all sites in
                 all states was requested.


DATA AVAILABLE FOR:


MOBILE AL              JUNEAU AK              PHOENIX AZ
LITTLE ROCK AR         LOS ANGELES CA         SACRAMENTO CA
SAN FRANCISCO CA       DENVER CO              HARTFORD CT
WILMINGTON DE          WASHINGTON DC          JACKSONVILLE FL
MIAMI FL               ATLANTA GA             HONOLULU HI
BOISE ID               CHICAGO IL             PEORIA IL
INDIANAPOLIS IN        DES MOINES IA          WICHITA KS
LOUISVILLE KY          NEW ORLEANS LA         PORTLAND ME
BALTIMORE MD           BOSTON MA              DETROIT MI
SAULT STE MARIE MI     DULUTH MN              MINNEAPOLIS/ST PAUL MN
JACKSON MS             KANSAS CITY MO         ST LOUIS MO
GREAT FALLS MT         OMAHA NB               RENO NV
CONCORD NH             ATLANTIC CITY NJ       ALBUQUERQUE NM
ALBANY NY              BUFFALO NY             NEW YORK NY
CHARLOTTE NC           RALEIGH NC             BISMARCK ND
CINCINNATI OH          CLEVELAND OH           COLUMBUS OH
OKLAHOMA CITY OK       PORTLAND OR            PHILADELPHIA PA
PITTSBURGH PA          PROVIDENCE RI          COLUMBIA SC
SIOUX FALLS SD         MEMPHIS TN             NASHVILLE TN
DALLAS/FORT WORTH TX   EL PASO TX             HOUSTON TX
SALT LAKE CITY UT      BURLINGTON VT          NORFOLK VA
RICHMOND VA            SEATTLE/TACOMA WA      SPOKANE WA
CHARLESTON WV          MILWAUKEE WI           CHEYENNE WY
SAN JUAN PR

Enter the name of the desired data site: [boston]


CURRENT SITE: BOSTON MA


Select run option: [help]


BACK         USE TO RETURN TO THE LIST OF SITES
BUILD        USE TO BUILD SESOIL/TOXSCREEN INPUT DATA FILES
REVIEW       USE TO REVIEW DATA FOR THE SELECTED SITE
EXIT         USE TO EXIT THE PROGRAM
```

```
CURRENT SITE: BOSTON MA

Select run option: [build]

                                  NOTE
                  ******************************
                  Request was made to build up the
                  SESOIL input data files from the
                  70-city database for the Boston
                  site.


Enter soil data option: [help]

DEFAULT     THE PROGRAM WILL SELECT AN APPROPRIATE SOIL
SPECIFIC    USER SELECTS A SOIL FROM SITE SPECIFIC SOILS
GENERIC     USER SELECTS A SOIL FROM A LIST OF GENERIC SOILS
BACK        TO RETURN TO THE PREVIOUS PROMPT
HELP        TO OBTAIN THESE HELP MESSAGES

Enter soil data option: [default]

                                  NOTE
                  ******************************
                  Request was made to let the
                  system automatically select an
                  appropriate soil which is one of
                  the needed SESOIL input information.


Do you wish to build a SESOIL data set for another location? [no]

                                  NOTE
                  ******************************
                  To simplify the illustration,
                  only one site (Boston) is
                  selected here.


Enter your name for the general data file: [gen]

Enter your name for the level data file: [lev]

                                  NOTE
                  ******************************
                  You can name the GENERAL and
                  LEVEL data files which contain
                  the data accessed from the
                  cities database.


** Database access completed **
```

```
Current GENERAL data file is : GEN
To use an alternate GENERAL data file,
enter the file name (<CR> for none)? [<CR>]

                              NOTE
                 ********************************
                 An option to let you call in
                 another GENERAL file to be used
                 instead of the newly created
                 file:GEN.DAT. <CR> indicates that
                 you want to bypass this option.

***** DETERMINATION OF SESOIL POLLUTANT APPLICATION LEVEL  *****

City DATABASE access

Selected SESOIL application level is :  3

                              NOTE
                 *********************************
                 Remember that the 70-city data-
                 base can be used to build up
                 files for LEVEL 3 study only.
                 For other Levels, select the
                 remaining two options (see Sec.III).

*****  AVAILABLE CLIMATIC REGIONS  *****


  1.  BOSTON MA                CANTON SANDY LOAM FINE S

Only one site is available ** automatically selected


*****  CLIMATOLOGICAL PARAMETERS  *****


  1.  L [deg N]    latitude of area
  2.  NAME

Enter data item to be updated : [review]

                              NOTE
                 ********************************
                 You are strongly recommended to
                 review all retrieved data to
                 check their validity.

You may review data for the current year or for all years available.
```

APP.1:SESOIL SAMPLE RUN FOR 1 YEAR USING BOTH SESIN AND SESOILFM(CONT'D)

```
Enter [C]urrent or [A]ll? [all]

                              NOTE
                 ********************************
                 Since there is only one year of
                 data presently available, the
                 entry of 'C' or 'A' makes no
                 difference.


   1 BOSTON MA                 CANTON SANDY LOAM FINE S     1
L       42.36
TA      13.00  7.330.5556 -1.56 -0.89  3.39  9.22 14.78 20.00 22.94 21.83 18.06
NN       0.53   0.6   0.6   0.6  0.56  0.56  0.58  0.58  0.57  0.56  0.53  0.51
S        0.57  0.61  0.61  0.57  0.57  0.57  0.53  0.57   0.6  0.56  0.57  0.61
A        0.18  0.21  0.28  0.37  0.35  0.28  0.21  0.18  0.18  0.18  0.18  0.18
REP      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
MPM      7.67 11.46 10.77  9.37  8.99 10.19  8.86  8.81  8.10  6.96  8.79  8.03
MTR    0.6667  1.040.7083 0.375  0.750.2917 0.3750.33330.20830.54170.0833   0.5
MN       7.00  4.00  9.00  6.00  8.00  5.00  9.00  7.00  8.00  9.00  5.00  7.00
MT       9.00 11.00 12.00 12.00 11.00 12.00 11.00 11.00 11.00  9.00 10.00  9.00

Press return to continue? [<CR>]

Enter data item to be updated : [done]

                              NOTE
                 ********************************
                 The use of 'done' signals that
                 the editing of the above data
                 has been completed and you are
                 advanced to the next prompt.


Current YEAR :  1

  1.  TA        [deg C]    temp of area
  2.  NN        [fraction] fraction of area covered by clouds
  3.  S         [fraction] relative humidity of area
  4.  A                    shortwave albedo of surface
  5.  REP       [cm/day]   dayly evapotranspiration or 0
  6.  MPM       [cm]       monthly precipitation
  7.  MTR       [days]     mean time of rain
  8.  MN        [#]        mean number of storm events
  9.  MT        [days]     mean length of rainy season

Enter data item to be updated : [1]

                              NOTE
                 ********************************
                 '1' means the values for TA are
                 to be updated.
```

```
The current values for TA        [deg C]    are

      1 Oct        2 Nov        3 Dec        4 Jan        5 Feb        6 Mar
      13.00         7.33   0.55559999        -1.56        -0.89         3.39

      7 Apr        8 May       9 June      10 July       11 Aug      12 Sept
       9.22        14.78        20.00        22.94        21.83        18.06

Enter the month(s) to alter? [10]

                              NOTE
                 ********************************
                 The value for July is to be
                 changed.


Enter the new value(s)? [24.0]

Current YEAR :  1

Enter data item to be updated : [done]

Would you like to enter data for another year? [no]

                              NOTE
                 ********************************
                 To simplify the illustration,
                 only one year of data is selected
                 here.  Multiple-year runs are
                 shown in Appendix 2.

*****  AVAILABLE SOILS  *****


  1.  CANTON SANDY LOAM FINE SANDY LOAM BOSTON

Only one soil is available ** automatically selected


*****  SOIL PARAMETERS  *****


  1.  RS      [g/cm2]   soil density
  2.  K1      [cm2]     soil intrinsic permeability
  3.  C                 soil disconnectedness index
  4.  N                 effective soil porosity
  5.  OC      [%oc]     organic content of soil
  6.  CC      [%cc]     clay content of soil
  7.  CEC     [me/100g] soil cation exchange capacity
  8.  K1U     [cm2]     intrinsic permeabilities of upper soil layer
  9.  K1M    [cm2]     intrinsic permeabilities of middle soil layer
 10.  K1L    [cm2]     intrinsic permeabilities of lower soil layer
 11.  RDUST  [ug/m3]   dust loading factor for TOXSCREEN only
 12.  NAME

Enter data item to be updated : [review]

                             NOTE
                  *******************************
                  Review is made here again to
                  to check the data.


   1 CANTON SANDY LOAM FINE SANDY LOAM BOSTON
     -  RS,K1,C,N,OC,CC                 1.35   0.00   6.00   0.26   0.00   0.00
     -  CDC,K1U,K1M,K1L,RDUST           0.00.288E-7.288E-7.936E-7   0.00

Press return to continue? [<CR>]

Enter data item to be updated : [5]

The current value for OC     is :    0.00 [%oc]
Enter the new value, or hit <CR> to leave the same : [0.20]

                             NOTE
                  *******************************
                  The value of OC is changed from
                  0.00 to 0.20.


Enter data item to be updated : [done]

*****  AVAILABLE CHEMICALS  *****


  1.  TEST CHEMICAL

Only one chemical is available ** automatically selected

*****  CHEMICAL PARAMETERS  *****


  1.  SL     [ug/mL]               compound solubility in water
  2.  KOC    [(ug/g oc)/(ug/mL)    adsorption coeff in organic carbon
  3.  DA     [cm2/sec]             diffusion coefficient in air
  4.  KDE    [day-1]               biodegradation rate of compound
  5.  H      [m3*atm/degK*mol]     Henrys Law constant
  6.  K      [(ug/g)/(ug/mL)]      averaged adsorption coeff for compound on soi
  7.  MWT    [g/mol]               molecular weight
  8.  VAL                          valence
  9.  KNH    [day-1]               neutral hydrolysis constant
 10.  KBH    [L/mol*day]           base hydrolysis constant
 11.  KAH    [L/mol*day]           acid hydrolysis constant
```

```
   12.  SK                          stability constant compound-ligand complex
   13.  B      [#]                  moles of ligand per mole of bound compound
   14.  MWTLIG [g/mol]              molecular weight of ligand
   15.  NAME

  Enter data item to be updated : [review]

     1 TEST CHEMICAL
       SL,KOC,DA,KDE,HENRY,K             730.00 157.00 0.0825  0.002 0.0031    0.00
       MWT,VAL,KNH,KBH,KAH               133.40   0.00   0.00   0.00   0.00
       SK,B,MWTLIG                         0.00   0.00   0.00

  Press return to continue? [<CR>]

  Enter data item to be updated : [all]

                                NOTE
                  ********************************
                  After review, changes to all of
                  the above data are requested.
                  The changes are carried out item
                  by item, as shown below.


                                NOTE
                  ********************************
                  Normally you would want to
                  replace the TEST CHEMICAL
                  parameters with your own
                  chemical data.


  The current name is : TEST CHEMICAL
  Enter the new name : [pcb-c12h9cl]

  The current value for SL     is :  730.00 [ug/mL]
  Enter the new value, or hit <CR> to leave the same : [1.17]

  The current value for KOC    is :  157.00 [(ug/g oc)/(ug/mL)
  Enter the new value, or hit <CR> to leave the same : [11500.0]

  The current value for DA     is :  0.0825 [cm2/sec]
  Enter the new value, or hit <CR> to leave the same : [0.06]

  The current value for KDE    is :   0.002 [day-1]
  Enter the new value, or hit <CR> to leave the same : [0.0346]

  The current value for H      is :  0.0031 [m3*atm/degK*mol]
  Enter the new value, or hit <CR> to leave the same : [0.0059]

  The current value for K      is :    0.00 [(ug/g)/(ug/mL)]
  Enter the new value, or hit <CR> to leave the same : [<CR>]
```

```
The current value for MWT    is :  133.40 [g/mol]
Enter the new value, or hit <CR> to leave the same : [<CR>]

The current value for VAL    is :    0.00
Enter the new value, or hit <CR> to leave the same : [<CR>]

The current value for KNH    is :    0.00 [day-1]
Enter the new value, or hit <CR> to leave the same : [<CR>]

The current value for KBH    is :    0.00 [L/mol*day]
Enter the new value, or hit <CR> to leave the same : [<CR>]

The current value for KAH    is :    0.00 [L/mol*day]
Enter the new value, or hit <CR> to leave the same : [<CR>]

The current value for SK     is :    0.00
Enter the new value, or hit <CR> to leave the same : [<CR>]

The current value for B      is :    0.00 [*]
Enter the new value, or hit <CR> to leave the same : [<CR>]

The current value for MWTLIG is :    0.00 [g/mol]
Enter the new value, or hit <CR> to leave the same : [<CR>]

Enter data item to be updated : [done]

Current application level data file is LEV
To use an alternate level data file,
enter the file name (<CR> for none)? [<CR>]

                              NOTE
                  ******************************
                  Editing of the GENERAL data file
                  has  been completed.  You are
                  now entering editing for the
                  LEVEL data file.


                              NOTE
                  ******************************
                  An option to let you call in
                  another LEVEL file to be used
                  instead of the newly created
                  file:LEV.DAT. <CR> indicates that
                  you want to bypass this option.


*****  AVAILABLE APPLICATION STUDY REGIONS  *****


  1.  BOSTON MA              CANTON SANDY LOAM FINE S
```

```
Only one site is available ** automatically selected


***** MODIFICATION OF ANNUAL APPLICATION PARAMETERS *****


  1.  AR     [cm2]   surface area
  2.  Z      [m]     depth to groundwater table
  3.  DU     [cm]    depth of upper unsaturated soil zone
  4.  DM     [cm]    depth of middle unsaturated soil zone
  5.  FRN            Freundlich equation exponent
  6.  PH             pH of upper unsaturated soil zone
  7.  A2PH           pH of middle unsaturated soil zone
  8.  APH            ratio: pH lower/upper unsaturated soil zone
  9.  A2KDE          ratio: biodeg rate lower/middle soil zone
 10.  AKDE           ratio: biodeg rate lower/upper soil zone
 11.  A2OC           ratio: organic carbon lower/middle
 12.  AOC            ratio: organic carbon lower/middle
 13.  A2CC           ratio: clay content lower/middle
 14.  ACC            ratio: clay content lower/upper
 15.  A2CEC          ratio: lower/middle soil zone cation exchange capacity
 16.  ACEC           ratio: lower/upper soil zone cation exchange capacity
 17.  NAME

Enter data item to be updated : [review]


You may review data for the current year or for all years available.
Enter [C]urrent or [A]ll? [all]


   1 BOSTON MA              CANTON SANDY LOAM FINE S    1
      - AR,Z,DU,DM,FRN                  10000.   2.74  15.24  68.58   1.00
      - PH,A2PH,APH                       4.80   1.00   1.00
      - A2KDE,AKDE,A2OC,AOC,A2CC,ACC      1.00   1.00   1.00   1.00   1.00   1.00
      - A2CEC,ACEC                        1.00   1.00
CUM       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
CMM       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
CLM       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
POLINU    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
POLINM    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
POLINL    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
ISRM      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
ASL       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANSU    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANSM    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
TRANSL    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINKU     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINKM     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
SINKL     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIGCU     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
LIGCM     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
```

```
LIGCL    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00

Press return to continue? [<CR>]

Enter data item to be updated : [done]

*****  MODIFICATION OF MONTHLY APPLICATION PARAMETERS  *****


Current YEAR :  1

  1.  CUM    [ug/mL]  conc pollutant in soil moisture upper zone
  2.  CMM    [ug/mL]  conc pollutant in soil moisture middle zone
  3.  CLM    [ug/mL]  conc pollutant in soil moisture lower zone
  4.  POLINU [ug/cm2] pollution load per unit area entering upper zone
  5.  POLINM [ug/cm2] pollution load per unit area entering middle zone
  6.  POLINL [ug/cm2] pollution load per unit area entering lower zone
  7.  ISRM   [ug/cm2] index for pollutant appearance in surface runoff
  8.  ASL             ratio: conc of pollutant/maximum solubility in H2O
  9.  TRANSU [ug/cm2] pollutant transformed in upper zone
 10.  TRANSM [ug/cm2] pollutant transformed in middle zone
 11.  TRANSL [ug/cm2] pollutant transformed in lower zone
 12.  SINKU  [ug/cm2] pollutant lost by processes not described (upper)
 13.  SINKM  [ug/cm2] pollutant lost by processes not described (middle)
 14.  SINKL  [ug/cm2] pollutant lost by processes not described (lower)
 15.  LIGU   [ug/cm2] ligand mass input to upper zone
 16.  LIGM   [ug/cm2] ligand mass input to middle zone
 17.  LIGL   [ug/cm2] ligand mass input to lower zone

Enter data item to be updated : [4]

The current values for POLINU [ug/cm2] are

      1 Oct       2 Nov       3 Dec       4 Jan       5 Feb       6 Mar
       0.00        0.00        0.00        0.00        0.00        0.00

      7 Apr       8 May       9 June     10 July     11 Aug     12 Sept
       0.00        0.00        0.00        0.00        0.00        0.00

Enter the month(s) to alter? [all]

                                  NOTE
                    ******************************
                    'all' allows you to change all
                    months with one constant value.


Enter the new value(s)? [5000.0]

Current YEAR :  1

Enter data item to be updated : [back]
```

```
                                NOTE
                   *********************************
                   'back' allows you to go back to
                   the the previous parameter group
                   for re-editing.


*****  MODIFICATION OF ANNUAL APPLICATION PARAMETERS  *****


   1.  AR      [cm2]     surface area
   2.  Z       [m]       depth to groundwater table
   3.  DU      [cm]      depth of upper unsaturated soil zone
   4.  DM      [cm]      depth of middle unsaturated soil zone
   5.  FRN               Freundlich equation exponent
   6.  PH                pH of upper unsaturated soil zone
   7.  A2PH              pH of middle unsaturated soil zone
   8.  APH               ratio: pH lower/upper unsaturated soil zone
   9.  A2KDE             ratio: biodeg rate lower/middle soil zone
  10.  AKDE              ratio: biodeg rate lower/upper soil zone
  11.  A2OC              ratio: organic carbon lower/middle
  12.  AOC               ratio: organic carbon lower/~~middle~~upper
  13.  A2CC              ratio: clay content lower/middle
  14.  ACC               ratio: clay content lower/upper
  15.  A2CEC             ratio: lower/middle soil zone cation exchange capacity
  16.  ACEC              ratio: lower/upper soil zone cation exchange capacity
  17.  NAME

Enter data item to be updated : [1]

The current value for AR     is :  10000. [cm2]
Enter the new value, or hit <CR> to leave the same : [1000.]

Enter data item to be updated : [brief]

                                NOTE
                   *********************************
                   'brief' suppresses the displaying
                   of the menu parameter descrip-
                   tions.  This will save editing
                   time for experienced users.


Enter data item to be updated : [done]

*****  MODIFICATION OF MONTHLY APPLICATION PARAMETERS  *****


Current YEAR :  1

   1.  CUM
   2.  CMM
   3.  CLM
```

```
        4.  POLINU
        5.  POLINM
        6.  POLINL
        7.  ISRM
        8.  ASL
        9.  TRANSU
       10.  TRANSM
       11.  TRANSL
       12.  SINKU
       13.  SINKM
       14.  SINKL
       15.  LIGU
       16.  LIGM
       17.  LIGL

   Enter data item to be updated : [done]

                          NOTE
                 ********************************
                 Since this data group has already
                 been edited, no additional
                 changes are made. (Notice that
                 the parameter descriptions are
                 suppressed.)

   Do you wish to enter data for additional years? [no]

                          NOTE
                 ********************************
                 A sample run for multiple years
                 of data is given in Appendix 2.

   Would you like to change any exec file parameters? [no]

                          NOTE
                 ********************************
                 Unless you are experienced in
                 the use of the EXEC file para-
                 meters, changes by you are not
                 recommended, except for making
                 multiple-year runs as shown in
                 Appendix 2.

   Would you like to enter data for another run? [no]

                          NOTE
                 ********************************
                 You are encouraged to try this
                 multiple run option.
```

APP.1:SESOIL SAMPLE RUN FOR 1 YEAR USING BOTH SESIN AND SESOILFM(CONT'D)

```
Current GENERAL new input default FILENAME is : GENERAL.DAT
Enter your new input FILENAME? [newgen]
```

NOTE
****
You can assign a specific name
to the just edited SESOIL-ready
GENERAL file. Here the name
NEWGEN.DAT was assigned. A <CR>
would have assigned the default
name: GENERAL.DAT.

```
Current Level 3 new input default filename is : LEVEL3.DAT
Enter the name for your new input file? [newlev]
```

NOTE
****
You can assign a specific name
to the just edited SESOIL-ready
LEVEL file. Here, the name
NEWLEV.DAT was assigned. A <CR>
would have assigned the default
name LEVEL3.DAT.

```
Do you want to run SESOIL: [yes]
```

NOTE
****
You have the option of running
SESOIL now(by responding 'yes')
or saving the newly edited data-
sets to be run at a later time
(a 'no' response).

```
Enter BATCH or INTERACTIVE : [i]
```

NOTE
****
You have the option to submit
a batch(b) or interactive(i) job.

```
Enter Y to output sesoil results to GEMS > [y]
```

NOTE
****
This is to indicate if the out-
put data management(SESOILFM)
support is requested or not.

```
   Enter GEMS output dataset name > [pcb]

                                  NOTE
                    *********************************
                    If SESOILFM support was requested
                    you need to give a name(1 to 12
                    characters) under which the output
                    dataset is to be stored in GEMS.


   Enter tag field > [sesoil run for pcb at boston]

                                  NOTE
                    *********************************
                    This is to give more descriptive
                    dataset identification.  Press
                    <CR> to bypass.


   DSNAME=TESTPCB1
    FMCLOS: IOPT=           1
  FORTRAN STOP

                                  NOTE
                    *********************************
                    At this point, SESOIL has been
                    successfully executed using the
                    two input files: NEWGEN.DAT and
                    NEWLEV.DAT.   The output file is
                    named SESOUT.DAT.


                                  NOTE
                    *********************************
                    At this point, SESOILFM has
                    stored selected SESOIL output
                    parameters into GEMS under the
                    name: PCB.  The link between
                    SESOIL and AT123D starts below.

  ENTER Y TO SEE SESOIL OUTPUT USABLE FOR AT123D > [y]

                                  NOTE
                    *********************************
                    'y' will allow you to review all
                    the AT123D-related SESOIL output
                    parameters prior to building up
                    an AT123D input file.  Those
                    assumptions which require special
                    consideration are displayed in
                    brackets.
```

APP.1:SESOIL SAMPLE RUN FOR 1 YEAR USING BOTH SESIN AND SESOILFM(CONT'D)

```
     THE FOLLOWING GIVES SELECTED SESOIL OUTPUTS AND
     THEIR CORRESPONDING AT123D INPUT VALUES
     (SEE USER'S GUIDE FOR ASSUMPTIONS MADE)


 (1)SESOIL-AREA(AR):   1000.000      SQ.CM.
    AT123D-SOURCE SIZE: RL1=  0.0000000E+00  RL2=  0.3162278
              (METERS)  RB1= -0.1581139      RB2=  0.1581139
                        RH1=  0.0000000E+00  RH2=  0.0000000E+00
 (2)SESOIL-EFFECTIVE POROSITY(N):  0.2600000
    AT123D-EFFECTIVE POROSITY(POR):  0.2600000
 (3)SESOIL-INTR. PERM.(K1):  5.5440285E-08  SQ. CM.
    AT123D-HYD. COND.(HCOND):  0.1710666      M/HR
  **[NOTE: POROSITY AND HYDR. COND. IN
    GROUNDWATER LAYERS MAY DIFFER SIGNIFICANTLY
    FROM THOSE USED IN SESOIL LAYERS.]
 (4)SESOIL-AD. COEF.(K):   23.00000      ML/G
    AT123D-DIS. COEF.(AKD):  2.3000002E-02  M**3/KG
  **[NOTE: K IS DETERMINED INDIRECTLY
    FROM KOC AND OC.]
  **[NOTE: ACTUAL VALUE OF AKD MAY BE LOWER
    DUE TO LOWER OC CONCENTRATION (<0.1%)
    IN GROUNDWATER LAYER OF AT123D.]
 (5)SESOIL-HYDROL. RATE(KNH):  0.0000000E+00  1/DAY
    AT123D-DECAY RATE(RAMADA):  0.0000000E+00  1/HR
  **[NOTE: OTHER PROCESSES IN ADDITION TO
    NEUTRAL HYDROLYSIS MAY BE CONSIDERED FOR
    TOTAL DEGREDATION IN GROUNDWATER.]
 (6)SESOIL-SOIL DENSITY(RS):   1.350000      G/CM**3
    AT123D-BULK DENSITY(RHOB):   1350.000      KG/M**3

 (7)SESOIL-MASS INTO GRW(12 VALUES PER YEAR)(KG/HR):

   1   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.2329E-11  0.4197E-11
       0.4553E-11  0.5116E-11  0.5013E-11  0.4576E-11  0.9528E-11  0.1260E-10

ENTER Y TO CREATE AT123D INPUT FILE
USING THE SELECTED SESOIL OUTPUTS > [y]

                               NOTE
                    ********************************
                    'y' allows you to create an
                    AT123D input file based on the
                    above SESOIL simulation run
                    outputs.
```

APP.1:SESOIL SAMPLE RUN FOR 1 YEAR USING BOTH SESIN AND SESOILFM(CONT'D)

```
ENTER THE DATA FILE NAME(6 CHARACTERS) > [pcb001]

                              NOTE
                 *******************************
                 An AT123D input data file name
                 has to be assigned here.
                 (6 characters are required.)


THE USABLE SESOIL VALUES HAVE BEEN STORED
IN AN AT123D INPUT DATASET:  pcb001.DAT
NOTE: THIS DATASET IS ALSO FILLED WITH OTHER
DEFAULT VALUES WHICH ARE TO BE USED WITH CAUTION.
YOU MAY EDIT THOSE DEFAULT VALUES USING AT123DIN.


DO YOU WANT TO RUN AT123D ?: [no]

                              NOTE
                 *******************************
                 'yes' will allow you to run
                 AT123D using AT123DIN and
                 AT123DOUT.  See the AT123D
                 User's Guide(GSC,1984).


ENTER AN OPERATION:

                               NOTE
                  *******************************
                  This is back to GEMS.
```

APPENDIX 2: SESOIL SAMPLE RUN FOR MULTIPLE YEARS USING SESIN

```
Enter an operation: [m]

Enter a model name: [sesoil]
Are you creating SESOIL input files: [yes]

                                   SESIN
                           INTERACTIVE SESOIL INPUT
                                 GSC VER1.1
                                  6-DEC-84

For a list of commands type : HELP COMMANDS


Do you want to use data from the cities database? [no]

Current GENERAL data file is : DBAO:[EEDDAL.DATA]GENERAL.DAT
To use an alternate GENERAL data file,
enter the file name (<CR> for none)? [newgen]

                            NOTE
                ******************************
                Here, the data file:NEWGEN.DAT
                created in Appendix 1 is called
                in instead of accessing the 70-
                cities database. (A <CR> entry
                to the last prompt would have
                accessed the default GENERAL data
                file shown in Appendix 4.


***** DETERMINATION OF SESOIL POLLUTANT APPLICATION LEVEL  *****

Are pollutant loadings available as monthly or annual data? [m]
Are there 2 or 3 unsaturated soil layers? [3]

                            NOTE
                ******************************
                The two above prompts determine
                the LEVEL type file used.

Selected SESOIL application level is :  3

*****  AVAILABLE CLIMATIC REGIONS  *****

  1.  BOSTON MA               CANTON SANDY LOAM FINE S

Only one site is available ** automatically selected
```

```
***** CLIMATOLOGICAL PARAMETERS *****


  1.  L [deg N]    latitude of area
  2.  NAME

Enter data item to be updated : [review]


You may review data for the current year or for all years available.
Enter [C]urrent or [A]ll? [all]


   1 BOSTON MA                CANTON SANDY LOAM FINE S    1
L       42.36
TA      13.00  7.330.5556 -1.56 -0.89  3.39  9.22 14.78 20.00 24.00 21.83 18.06
NN       0.53   0.6   0.6   0.6  0.56  0.56  0.58  0.58  0.57  0.56  0.53  0.51
S        0.57  0.61  0.61  0.57  0.57  0.57  0.53  0.57   0.6  0.56  0.57  0.61
A        0.18  0.21  0.28  0.37  0.35  0.28  0.21  0.18  0.18  0.18  0.18  0.18
REP      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
MPM      7.67 11.46 10.77  9.37  8.99 10.19  8.86  8.81  8.10  6.96  8.79  8.03
MTR    0.6667  1.040.7083 0.375  0.750.2917 0.3750.33330.20830.54170.0833   0.5
MN       7.00  4.00  9.00  6.00  8.00  5.00  9.00  7.00  8.00  9.00  5.00  7.00
MT       9.00 11.00 12.00 12.00 11.00 12.00 11.00 11.00 11.00  9.00 10.00  9.00


Press return to continue? [<CR>]

Enter data item to be updated : [brief]

                              NOTE
                 ********************************
                 'brief' is used for more efficient
                 editing.


Enter data item to be updated : [done]

Current YEAR :  1

  1.  TA
  2.  NN
  3.  S
  4.  A
  5.  REP
  6.  MPM
  7.  MTR
  8.  MN
  9.  MT

Enter data item to be updated : [done]
```

```
Would you like to enter data for another year? [yes]
The previous years data is available.  Do you wish to use it? [yes]

                         NOTE
                 *********************************
                 A second year of data for the
                 GENERAL file is generated by
                 repeating the first year of data.


Current YEAR :  2

  1.  TA
  2.  MN
  3.  S
  4.  A
  5.  REP
  6.  MPM
  7.  MTR
  8.  MN
  9.  MT

Enter data item to be updated : [done]

                         NOTE
                 *********************************
                 This second year of GENERAL data
                 can be edited.  Here, no changes
                 are made.


Would you like to enter data for another year? [no]

                         NOTE
                 *********************************
                 Additional years of data can be
                 generated in the same way up to
                 10 years.  Here, only one addi-
                 tional year has been generated.

*****  AVAILABLE SOILS  *****


  1.  CANTON SANDY LOAM FINE SANDY LOAM BOSTON

Only one soil is available ** automatically selected


*****  SOIL PARAMETERS  *****
```

```
   1.  RS
   2.  K1
   3.  C
   4.  N
   5.  OC
   6.  CC
   7.  CEC
   8.  K1U
   9.  K1M
  10.  K1L
  11.  RDUST
  12.  NAME

Enter data item to be updated : [done]

*****  AVAILABLE CHEMICALS  *****


   1.  PCB-C12H9CL

Only one chemical is available ** automatically selected

*****  CHEMICAL PARAMETERS  *****


   1.  SL
   2.  KOC
   3.  DA
   4.  KDE
   5.  H
   6.  K
   7.  MWT
   8.  VAL
   9.  KNH
  10.  KBH
  11.  KAH
  12.  SK
  13.  B
  14.  MWTLIG
  15.  NAME

Enter data item to be updated : [review]


    1 PCB-C12H9CL
      SL,KOC,DA,KDE,HENRY,K                 1.17 11500.    0.06 0.0346 0.0059    0.00
      MWT,VAL,KNH,KBH,KAH                 133.40    0.00    0.00   0.00   0.00
      SK,B,MWTLIG                           0.00    0.00    0.00

Press return to continue? [<CR>]

Enter data item to be updated : [done]
```

```
                              NOTE
                    ********************************
                    No changes have been made to any
                    of the GENERAL data paramters.


   Current application level data file is DBA0:[EEDDAL.DATA]LEVEL3.DAT
   To use an alternate level data file,
   enter the file name (<CR> for none)? [newlev]

                              NOTE
                    ********************************
                    Here, the data file:NEWLEV.DAT
                    created in the sample run in
                    Appendix 1 is called in instead
                    of accessing the 70-cities data-
                    base.  (A <CR> entry would have
                    accessed one of the default level
                    data files shown in Appendix 4.)


   *****  AVAILABLE APPLICATION STUDY REGIONS  *****


     1.  BOSTON MA              CANTON SANDY LOAM FINE S


   Only one site is available ** automatically selected


   *****  MODIFICATION OF ANNUAL APPLICATION PARAMETERS  *****


     1.  AP
     2.  Z
     3.  DU
     4.  DM
     5.  FRN
     6.  PH
     7.  A2PH
     8.  APH
     9.  A2KDE
    10.  AKDE
    11.  A2OC
    12.  AOC
    13.  A2CC
    14.  ACC
    15.  A2CEC
    16.  ACEC
    17.  NAME

   Enter data item to be updated : [done]
```

APP.2: SESOIL SAMPLE RUN FOR MULTIPLE YEARS USING SESIN(CONT'D)

```
*****  MODIFICATION OF MONTHLY APPLICATION PARAMETERS  *****

Current YEAR :  1

   1.  CUM
   2.  CMM
   3.  CLM
   4.  POLINU
   5.  POLINM
   6.  POLINL
   7.  ISRM
   8.  ASL
   9.  TRANSU
  10.  TRANSM
  11.  TRANSL
  12.  SINKU
  13.  SINKM
  14.  SINKL
  15.  LIGU
  16.  LIGM
  17.  LIGL

Enter data item to be updated : [review]


You may review data for the current year or for all years available.
Enter [C]urrent or [A]ll? [all]


   1 BOSTON MA                 CANTON SANDY LOAM FINE S    1
     - AR,Z,DU,DM,FRN                     10000.    2.74  15.24  68.58   1.00
     - PH,A2PH,APH                          4.80    1.00   1.00
     - A2KDE,AKDE,A2OC,AOC,A2CC,ACC         1.00    1.00   1.00   1.00   1.00   1.00
     - A2CEC,ACEC                           1.00    1.00
CUM       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
CMM       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
CLM       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
POLINU   5000.  5000.  5000.  5000.  5000.  5000.  5000.  5000.  5000.  5000.  5000.  5000.
POLINM    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
POLINL    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
ISRM      0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
ASL       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
TRANSU    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
TRANSM    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
TRANSL    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
SINKU     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
SINKM     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
SINKL     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
LIGCU     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
LIGCM     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
LIGCL     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
```

```
Press return to continue? [<CR>]

Current YEAR :  1

Enter data item to be updated : [done]
Do you wish to enter data for additional years? [yes]
The previous years data is available.  Do you wish to use it? [yes]


                           NOTE
                 *********************************
                 A second year of data for the
                 LEVEL data file is generated by
                 repeating the first year of data.


*****  MODIFICATION OF MONTHLY APPLICATION PARAMETERS  *****


Current YEAR :  2

  1.  CUM
  2.  CMM
  3.  CLM
  4.  POLINU
  5.  POLINM
  6.  POLINL
  7.  TSRM
  8.  ASL
  9.  TRANSU
 10.  TRANSM
 11.  TRANSL
 12.  SINKU
 13.  SINKM
 14.  SINKL
 15.  LIGU
 16.  LIGM
 17.  LIGL

Enter data item to be updated : [nobrief]

                           NOTE
                 *********************************
                 'nobrief' turns off the 'brief'
                 command and all parameter descri-
                 ptions will be displayed.


Current YEAR :  2

Enter data item to be updated : [done]
```

```
                              NOTE
                   *********************************
                   No changes have been made to the
                   generated second year of LEVEL
                   data.


   Do you wish to enter data for additional years? [no]

                              NOTE
                   *********************************
                   Note that the number of years of
                   data in the GENERAL and LEVEL
                   data files must be the same.


   Would you like to change any exec file parameters? [yes]

                              NOTE
                   *********************************
                   A 'yes' response here displays
                   the EXEC file menu for editing.


     1.  JRUN    Do Not Change!
     2.  LEVEL   level of operation
     3.  JRE     index of area of application (GENERAL file)
     4.  JSO     soil index
     5.  JCH     chemical index
     6.  JNUT    nutrient cycle (cannot change)
     7.  JAPPL   application area (LEVEL file)
     8.  JYRS    number of years to be simulated (must be 1 for annual)

   Enter data item to be updated : [8]

   The current value for JYRS  is :    2.00
   Enter the new value, or hit <CR> to leave the same : [5]

                              NOTE
                   *********************************
                   Here, it is desired to increase
                   the number of years to be simulated
                   from 2 to 5.  Because only 2 years
                   of data are available (as previously
                   created), the auxiliary pollution
                   load data file is created as follows.
                   (This is the decision to enter
                   Branch 1-A:See Fig. 1)
```

```
                                   NOTE
                         *********************************
                         This method of generating addi-
                         tional data is usually used for
                         long periods of simulation.  Up
                         to 100 years may be simulated.
                         Note that only the pollution
                         load parameters (POLINU,POLINM,
                         and POLINL) are edited.  The
                         remaining GENERAL and LEVEL data
                         parameters are automatically
                         generated based on repeated use
                         of the last year of available data.


   Enter data item to be updated : [done]

   AUX LOADINGS FILE

   You have 2 years of data.
   you must enter 3 more years.


     1.  SAME        sets all elements to the same number
     2.  RECYCLE     recycles existing loading data for remaining yea
     3.  EDIT        normal SESIN data entry/editing procedures

                                   NOTE
                         *********************************
                         Two options are available for
                         generating the auxiliary loading
                         data file.(Option no. 2 has not
                         yet been implemented in the
                         present version.)


   Enter method of loading entry: [1]

                                   NOTE
                         *********************************
                         The 'SAME' method of generating
                         loading data repeats a 1-year
                         loading scenario for all the
                         additional years of data required.

   Enter soil layer (1, 2, or 3)? [1]

                                   NOTE
                         *********************************
                         Here, the loading is applied to
                         the upper soil layer (layer 1),
                         (POLINU).
```

```
Enter month(s) to alter? [all]

                           NOTE
                ********************************
                Here, all months in a year will
                have the same loading value.


Enter loading? [2000.]


                           NOTE
                ********************************
                Here, a loading value of 2000 is
                applied to all months of all of
                the remaining years required
                (years 3,4 and 5).

You have 5 years of data.
you must enter 0 more years.


  1.  SAME       sets all elements to the same number
  2.  RECYCLE    recycles existing loading data for remaining yea
  3.  EDIT       normal SESIN data entry/editing procedures

Enter method of loading entry: [3]

                           NOTE
                ********************************
                The 'EDIT' method of loading data
                entry allows you to edit the
                loading quantities for individual
                years.


*****  ENTRY OF AUXILARY LOADING PARAMETERS  *****


Current YEAR :  3

  1.  POLINU     Upper level loadings
  2.  POLINM     middle level loadings
  3.  POLINL     lower level loadings

                           NOTE
                ********************************
                Editing begins with the first
                year in the AUX loading file
                (year 3).
```

```
Enter data item to be updated : [1]

                              NOTE
                    ********************************
                    Here, the source load is applied
                    to the upper soil layer (POLINU).


The current values for POLINU    are

     1 Oct       2 Nov       3 Dec       4 Jan       5 Feb       6 Mar
   2000.00     2000.00     2000.00     2000.00     2000.00     2000.00

     7 Apr       8 May      9 June     10 July      11 Aug     12 Sept
   2000.00     2000.00     2000.00     2000.00     2000.00     2000.00

Enter the month(s) to alter? [done]

                              NOTE
                    ********************************
                    No months are to be altered.


Current YEAR :  3

Enter data item to be updated : [next]

                              NOTE
                    ********************************
                    'next' advances the editing to
                    the next year.


Current YEAR :  4

Enter data item to be updated : [1]

The current values for POLINU    are

     1 Oct       2 Nov       3 Dec       4 Jan       5 Feb       6 Mar
   2000.00     2000.00     2000.00     2000.00     2000.00     2000.00

     7 Apr       8 May      9 June     10 July      11 Aug     12 Sept
   2000.00     2000.00     2000.00     2000.00     2000.00     2000.00

Enter the month(s) to alter? [all]
Enter the new value(s)? [1000.]

                              NOTE
                    ********************************
                    Here, the values of POLINU for
                    all months of year 4 are changed
```

APP.2: SESOIL SAMPLE RUN FOR MULTIPLE YEARS USING SESIN(CONT'D)

```
                    from 2000 to 1000.

     Current YEAR :  4

     Enter data item to be updated : [done]

                                   NOTE
                    ********************************
                    No more changes are to be made
                    for year 4.


     You have 5 years of data.
     you must enter 0 more years.


       1.  SAME      sets all elements to the same number
       2.  RECYCLE   recycles existing loadings data for remaining years
       3.  EDIT      normal SESIN data entry/editing procedures

     Enter method of loading entry: [done]

                                   NOTE
                    ********************************
                    Here, 'done' indicates that you
                    have completed all editing of
                    the auxiliary loading data file
                    AUX.


     Would you like to enter data for another run? [no]

     Current GENERAL new input default FILENAME is : GENERAL.DAT
     Enter your new input FILENAME? [newgen2]
     Current Level 3 new input default filename is : LEVEL3.DAT
     Enter the name for your new input file? [newlev2]
     Enter filename for aux loadings file: [aux5]

                                   NOTE
                    ********************************
                    You must also specify a filename
                    for the auxiliary loading file.


     Do you want to run SESOIL: [yes]

     Enter BATCH or INTERACTIVE : [b]
      Enter Y to output sesoil results to GEMS > [<CR>]
      Job 9410 entered on queue SYS BATCH
```

APP.2: SESOIL SAMPLE RUN FOR MULTIPLE YEARS USING SESIN(CONT'D)

```
                             NOTE
                ******************************* 
                Here, the run is submitted as a
                batch job.


Enter an operation:

                             NOTE
                *******************************
                This is back to GEMS.
```

APPENDIX 3: SESOIL SAMPLE RUN BYPASSING BOTH SESIN AND SESOILFM

```
    Enter an operation: [m]

    Enter a model name: [sesoil]
    Are you creating SESOIL input files: [no]

                                  NOTE
                         *******************************
                         This is the decision to enter
                         either Branch 1 or Branch 2(See
                         Fig. 1).  This example shows
                         that Branch 2(i.e. no SESIN
                         support) has been requested.


    Enter DUMMY below if the file(s) is not needed
    by your run

    Enter filename of GENERAL data file:  [newgen]
    Enter filename of LEVEL0 data file:  [dummy]
    Enter filename of LEVEL1 data file:  [dummy]
    Enter filename of LEVEL2 data file:  [dummy]
    Enter filename of LEVEL3 data file:  [newlev]
    Enter filename of EXEC data file:  [exec]
    Enter filename of AUXILIARY data file(needed if JYRS>run years):  [dummy]

                                  NOTE
                         *******************************
                         Since SESIN support is not
                         requested, the above are to input
                         your own GENERAL, LEVEL, and EXEC
                         data files.  Only one LEVEL file
                         is needed for each run.  The
                         AUXILIARY data file is needed if
                         the value of JYRS in the EXEC
                         file is greater than the number
                         of years of data available in
                         the GENERAL and LEVEL files
                         (see Appendix 2).

     Enter BATCH or INTERACTIVE : [i]

     Enter Y to output SESOIL results to GEMS > [<CR>]

                                  NOTE
                         *******************************
                         <CR> indicates that SESOILFM
                         support is not requested.
     DSNAME=-1
      FMCLOS: IOPT=           0
    FORTRAN STOP
```

APP.3:SESOIL SAMPLE RUN BYPASSING BOTH SESIN AND SESOILFM(CONT'D)

```
                            NOTE
                 *********************************
                 Indication of SESOIL FORTRAN
                 execution completion.


ENTER Y TO SEE SESOIL OUTPUT USABLE FOR AT123D > [<CR>]

                            NOTE
                 *********************************
                 Review of SESOIL output usable
                 for AT123D is not requested.


ENTER Y TO CREATE AT123D INPUT FILE
USING THE SELECTED SESOIL OUTPUTS > [<CR>]

                            NOTE
                 *********************************
                 Build up of AT123D input file
                 via SESOIL output is not requested.


DO YOU WANT TO RUN AT123D ?: [no]

The output file for this modeling run is named SESOUT.DAT
Enter rename, print, type or <CR> to exit: [<CR>]

                            NOTE
                 *********************************
                 Here, the decision is to exit.



Enter a model name:

                            NOTE
                 *********************************
                 This is back to GEMS.



********************************NOTE********************************
********************************************************************
In summary, this example shows a SESOIL run without the support
of SESIN and SESOILFM.  The user needs to input his own data
files.  The complete SESOIL output is stored in a file named
SESOUT.DAT.
********************************************************************
```

APPENDIX 4: SESIN-PROVIDED DEFAULT DATA FILES: GENERAL, LEVEL0, LEVEL1, LEVEL2, AND LEVEL3

GENERAL DATA FILE

```
1      REGIONAL DESCRIPTIONS; CLIMATIC,STORM DATA: (TEST DATA ONLY)
    1 CLINTON,    MA. (SUB-HUMID):
       -  L,TA,NN,S,A,REP                  42.50    8.40    0.35    0.70    0.30    0.00
       -  MPA,MTR,MN,HT                    94.10    0.32  109.00  365.00
       -  MP(M) (OCTOBER-MARCH)            10.36    8.96   12.52   11.75    8.33    8.33
       -  MP(M) (APRIL-SEPTEMBER)           8.38    7.82    6.60    5.08    6.04    8.46
    2 SITE B (MONTANA) (1940-1979)
       -  L,TA,NN,S,A,REP                  45.00   10.05    0.30     .55    0.25    0.00
       -  MPA,MTR,MN,MT                    36.74    0.24   103.0  365.00
       -  MP(M)OCT-MAR                      2.00    1.63    2.59    4.11    5.44    6.25
       -  MP(M)APR-SEP                      2.33    2.36    3.40    2.84    1.96    1.83
    3 SITE A (KANSAS) (1940-1980)
       -  L,TA,NN,S,A,REP                  39.00   14.30    0.30    60.0    0.10    0.00
       -  MPA,MTR,MN,MT                    84.83    0.20   105.0  365.00
       -  MP(M)OCT-MAR                      6.40    4.22    2.95    2.46    3.20    5.20
       -  MP(M)APR-SEP                      7.82   11.10   12.17    9.97   10.24    9.12
    4 CLINTON,MASS.(40 YR AVERAGED DATA FOR TEST ONLY)   10
 L         42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50
 TA         8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40
 NN          .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32
 S           .70   .70   .70   .70   .70   .70   .70   .70   .70   .70   .70   .70
 A          0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3
 REP        0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
 MPM        7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84
 MTR         .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32
 MN         9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08
 MT        30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42

 L-2       42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50
 TA-2       8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40
 NN-2        .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32
 S-2         .70   .70   .70   .70   .70   .70   .70   .70   .70   .70   .70   .70
 A-2        0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3
 REP-2      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
 MPM-2      7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84
 MTR-2       .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32
 MN-2       9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08
 MT-2      30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42

 L-3       42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50
 TA-3       8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40
 NN-3        .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32
 S-3         .70   .70   .70   .70   .70   .70   .70   .70   .70   .70   .70   .70
 A-3        0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3
 REP-3      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
 MPM-3      7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84
```

APP. 4: SESIN-PROVIDED DEFAULT DATA FILES (CONT'D)

```
MTR-3     .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32
MN-3     9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08
MT-3    30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42

L-4     42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50
TA-4     8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40
NN-4      .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32
S-4       .70    .70    .70    .70    .70    .70    .70    .70    .70    .70    .70    .70
A-4      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
REF-4    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
MPM-4    7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84
MTR-4     .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32
MN-4     9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08
MT-4    30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42

L-5     42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50
TA-5     8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40
NN-5      .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32
S-5       .70    .70    .70    .70    .70    .70    .70    .70    .70    .70    .70    .70
A-5      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
REF-5    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
MPM-5    7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84
MTR-5     .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32
MN-5     9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08
MT-5    30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42

L-6     42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50
TA-6     8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40
NN-6      .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32
S-6       .70    .70    .70    .70    .70    .70    .70    .70    .70    .70    .70    .70
A-6      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
REF-6    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
MPM-6    7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84
MTR-6     .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32
MN-6     9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08
MT-6    30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42

L-7     42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50
TA-7     8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40
NN-7      .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32
S-7       .70    .70    .70    .70    .70    .70    .70    .70    .70    .70    .70    .70
A-7      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
REF-7    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00
MPM-7    7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84   7.84
MTR-7     .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32
MN-7     9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08   9.08
MT-7    30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42  30.42

L-8     42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50  42.50
TA-8     8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40   8.40
NN-8      .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32    .32
S-8       .70    .70    .70    .70    .70    .70    .70    .70    .70    .70    .70    .70
A-8      0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3    0.3
```

```
REP-8     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
MPM-8     7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84
MTR-8      .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32
MN-8      9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08
MT-8     30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42

L-9      42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50
TA-9      8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40
NN-9       .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32
S-9        .70   .70   .70   .70   .70   .70   .70   .70   .70   .70   .70   .70
A-9       0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3
REP-9     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
MPM-9     7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84
MTR-9      .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32
MN-9      9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08
MT-9     30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42

L-10     42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50 42.50
TA-10     8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40  8.40
NN-10      .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32
S-10       .70   .70   .70   .70   .70   .70   .70   .70   .70   .70   .70   .70
A-10      0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3   0.3
REP-10    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
MPM-10    7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84  7.84
MTR-10     .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32   .32
MN-10     9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08  9.08
MT-10    30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42


2     SOIL CLASSIFICATION DATA: (TEST DATA ONLY)
   1 CLAY
       -  RS,K1,C,N,OC,CC                 1.32 1.E-10  12.00   0.45   1.46
       -  CEC,K1U,K1M,K1L                15.00   0.00   0.00   0.00
   2 SILTY-LOAM-KANSAS
       - RS,K1,C,N,OC,CC                  1.32 7.E-09   6.00   0.35    2.9
       - CEC                              0.00
   3 SILTY-CLAY-MONTANA
       - RS,K1,C,N,OC,CC                  1.324.2E-10  10.00   0.35    .63
       - CEC                              0.00
   4 SILTY-LOAM-KANSAS (K1 ADJUSTED)
       -  RS,K1,C,N,OC,CC                 1.32 1.E-13   6.00   0.35    2.9
       -  CEC                             0.00
   5 CLAY-LOAM GENERIC
      -RS,K1,C,N,OC,CC                    1.32 .28E-9  10.00   0.35    1.3 .20E-1
      -CEC                                 .00
   6 SANDY-LOAM
       -  RS,K1,C,N,OC,CC                 1.322.5E-10   4.00   0.25   0.10   0.00
       -  CEC                             0.00
   7 TEST SOIL
       -  RS,K1,C,N,OC,CC                 1.32 .25E-9   4.00   0.25   0.10   5.00
       -  CEC,K1U,K1M,K1L                15.00 .22E-9 .33E-9 .44E-9
   8 SILTY-LOAM GENERIC
```

APP. 4: SESIN-PROVIDED DEFAULT DATA FILES (CONT'D)

```
          -RS,K1,C,N,OC,CC                     1.32 1.2E-9   6.00   0.35    2.9
          -CEC                                 0.00
       9 SAND-GENERIC
          -RS,K1,C,N,OC,CC                     1.32 1.0E-7   3.50   0.25    .01
          -CEC                                 0.00
   3      CHEMISTRY DATA;   (TEST DATA ONLY)   Please review & modify before use!
       1 COPPER
         SL,KOC,DA,KDE,H,K                     0.00   0.00   0.00   0.00   0.00  10.00
         MWT,VAL,KNH,KBH,KAH                   0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
       2 SODIUM
         SL,KOC,DA,KDE,H,K                     0.00   0.00   0.00   0.00   0.00    .10
         MWT,VAL,KNH,KBH,KAH                   0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
       3 CHROMIUM
         SL,KOC,DA,KDE,H,K                     0.00   0.00   0.00   0.00   0.00 250.00
         MWT,VAL,KNH,KBH,KAH                   0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
       4 NICKEL
         SL,KOC,DA,KDE,H,K                     0.00   0.00   0.00   0.00   0.00   2.50
         MWT,VAL,KNH,KBH,KAH                   0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
       5 NAPTHALENE
         SL,KOC,DA,KDE,H,K                     0.0 1070.006.98E-6   0.00   0.00   0.00
         MWT,VAL,KNH,KBH,KAH                   0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
       6 ANTHRACENE
         SL,KOC,DA,KDE,H,K                     0.00   1.6E45.89E-6   0.00   0.00    .00
         MWT,VAL,KNH,KBH,KAH                   0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
       7 SODIUM-ADJUSTED KOC
         SL,KOC,DA,KDE,H,K                     0.00   0.00   0.00   0.00   0.00   1.00
         MWT,VAL,KNH,KBH,KAH                   0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
       8 PERCHLOROETHLYENE(=TETRACHLOROETHLYENE)
         SL,KOC,KD,KDE,HENRY,K               150.00 468.00  .0746   0.00 .00204   0.00
         MWT,VAL,KNH,KBH,KAH,MWTLIG            0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
       9 1,1,1-TRICHLOROETHANE
         SL,KOC,DA,KDE,HENRY,K               720.00 174.00  .0803   0.00 .00298   0.00
         MWT,VAL,KNH,KBH,KAH,MWTLIG            0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
      10 METHLYCHLOROFORM
         SL,KOC,DA,KDE,HENRY,K               730.00 189.00  .0825   0.00 .00231   0.00
         MWT,VAL,KNH,KBH,KAH,MWTLIG            0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
      11 METHLYENE CHLORIDE
         SL,KOC,DA,KDE,HENRY,K               13200.  11.00  .1033   0.003.68E-4   0.00
         MWT,VAL,KNH,KBH,KAH,MWTLIG            0.00   0.00   0.00   0.00   0.00   0.00
         SK,B,MWTLIG                           0.00   0.00   0.00   0.00   0.00   0.00
      12 CARBON TETRACHLORIDE
         SL,KOC,DA,KDE,HENRY,K               785.00 269.00  .0828   0.00 .00232   0.00
         MWT,VAL,KNH,KBH,KAH,MWTLIG          B 0.00   0.00   0.00   0.00   0.00   0.00
```

APP. 4: SESIN-PROVIDED DEFAULT DATA FILES (CONT'D)

```
     SK,B,MWTLIG                       0.00   0.00   0.00   0.00   0.00   0.00
  13 FREON 113
     SL,KOC,DA,KDE,HENRY,K           170.00 642.00  .0693   0.00   .391   0.00
     MWT,VAL,KNH,KBH,KAH,MWTLIG        0.00   0.00   0.00   0.00   0.00   0.00
     SK,B,MWTLIG                       0.00   0.00   0.00   0.00   0.00   0.00
  14 TRICHLOROETHYLENE(TCE)
     SL,KOC,DA,KDE,HENRY,K          1100.00 100.00  .0830   0.009.44E-3   0.00
     MWT,VAL,KNH,KBH,KAH,MWTLIG        0.00   0.00   0.00   0.00   0.00   0.00
     SK,B,MWTLIG                       0.00   0.00   0.00   0.00   0.00   0.00
  15 TEST CHEM
     SL,KOC,DA,KDE,HENRY,K          1100.00 360.00 8.3E-6   0.2 9.44E-3
     MWT,VAL,KNH,KBH,KAH               5.00   2.00  .7E-5   8.00   9.00  10.00
     SK,B,MWTLIG                    100000.   2.00  10.00   0.00   0.00   0.00
9    END FILE
```

LEVELO DATA FILE

```
   1 CLINTON,    MA. (SUB-HUMID):  FLAG
       -  AR,Z,DU,PH,APH                1.00 100.0   15.00   7.00   1.00
       -  AKDE,AOC,ACC,ISRA,ASL,ACEC     .50    .50   0.50   1.00   .001
       -  POLINU,POLINL,LIGU,LIGL      200.0 1000.0 1000.0 2000.0
       -  THA,INF,RGA,RSA              25.7   60.70  26.2   33.9
   2 TEST LOCATION
       -  AR,Z,DU,PH,APH                1.00 100.00  15.00   8.00   .875
       -  AKDE,AOC,ACC,ISRA,ASL,ACEC    1.10   1.20   1.30    .40   0.5    .001
       -  POLINU,POLINL,LIGC,ALIGC    200.00 1000.0  10.00  50.00
       -  THA,IA,RGA,RSA               25.70  60.70  26.20  33.90
9    END FILE
```

LEVEL1 DATA FILE

```
   1 CLINTON,    MA. (SUB-HUMID):
       -  AR,Z,DU,PH,APH                1.00 100.0   15.00   7.00   1.00
       -  AKDE,AOC,ACC,ISRA,ASL,ACEC     .50    .50   0.50   1.00   .001
       -  SPOLI,SPOLL,LIGU,LIGL        200.0 1000.0 1000.0 2000.0
   2 TEST LOCATION
       -  AR,Z,DU,PH,APH               10.00 100.00  15.00   8.00   .875
       -  AKDE,AOC,ACC,ISRA,ASL,ACEC    1.10   1.20   1.30    .40   0.5    .001
       -  POLINU,POLINL,LIGC-LIGL     200.00 1000.0  10.00  50.00
9    END OF FILE
```

LEVEL2 DATA FILE

```
    1 KANSAS-COPPER  (OCT. '78-SEP '80)                         2
         -  AR,Z,DU,PH,APH                      1.00  50.0    15.00
         -  AKDE,ADC,ACC,FRN,ACEC               0.00   1.00    0.00   1.00   0.00
 CUM       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 CLM       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 POLINU    0.00  0.00  0.00  0.00  0.00  0.00  3.24  0.00  0.00  0.00  0.00  0.0
 POLINL    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 ISRM      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 ASL       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 TRANSU    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 TRANSL    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 SINKU     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 SINKL     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 LIGU      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 LIGL      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 CUM2      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 CLM2      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 POLINU2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 POLINL2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 ISRM2     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 ASL2      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 TRANSU2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 TRANSL2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 SINKU2    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 SINKL2    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 LIGU2     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 LIGL2     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
    2 TEST RUN (CLINTON, MA. 40 YEARS)                          5
         -  AR,Z,DU,PH,APH                      1.00 100.00  15.00   8.00   .875
         -  AKDE,ADC,ACC,FRN,ACEC               1.10   1.20   1.30   1.40   .001
 CUM       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 CLM       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 POLINU  200.0   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 POLINU 1000.0   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 ISRM      1.00  1.00  1.00  1.00  1.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 TRANSU    0.20  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 TRANSL    0.30  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 SINKU     0.40  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 SINKL     0.50  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 LIGU   1000.0   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 LIGL   2000.0   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 CUM2      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 CLM2      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 POLINU2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 POLINL2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
 ISRM2     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
```

```
        ASL2     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        TRANSU2  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        TRANSL2  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        SINKU2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        SINKL2   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        LIGU2    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        LIGL2    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        CUM3     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        CLM3     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        FOLINU3  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        FOLINL3  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        ISRM3    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        ASL3     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        TRANSU3  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        TRANSL3  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        SINKU3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        SINKL3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        LIGU3    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        LIGL3    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        CUM4     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        CLM4     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        FOLINU4  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        FOLINL4  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        ISRM4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        ASL4     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        TRANSU4  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        TRANSL4  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        SINKU4   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        SINKL4   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        LIGU4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        LIGL4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        CUM5     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        CLM5     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        FOLINU5  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        FOLINL5  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        ISRM5    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        ASL5     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        TRANSU5  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        TRANSL5  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        SINKU5   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        SINKL5   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        LIGU5    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
        LIGL5    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
       9      END FILE
```

LEVEL3 DATA FILE

```
    1 TEST RUN                                            10
      -AR,Z,DU,DM,FRN                      1.00 100.00 15.00   0.01   1.40
      -PH,A2PH,APH                         8.00   1.00  .875
      -A2KDE,AKDE,A2OC,AOC,A2CC,ACC        1.10   1.10  1.20   1.20   1.30   1.30
      -A2CEC,ACEC                          1.30   1.30
 CUM       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 CMM       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 CLM       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 POLINU  200.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 POLINM    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 POLINL  1000.0   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 ISRM      1.00   1.00   1.00   1.00   1.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 ASL       .001   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 TRANSU    0.20   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 TRANSM    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 TRANSL    0.30   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 SINKU     0.40   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 SINKM     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 SINKL     0.50   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 LIGCU   1000.0   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 LIGCM     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 LIGCL   2000.0   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 CUM-2     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 CMM-2     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 CLM-2     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 POLINU2   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 POLINM2   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 POLINL2   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 ISRM-2    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 ASL-2     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 TRANSU    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 TRANSM    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 TRANSL    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 SINKU2    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 SINKM2    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 SINKL2    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 LIGCU2    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 LIGCM2    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 LIGCL2    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 CUM-3     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 CMM-3     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 CLM-3     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 POLINU3   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 POLINM3   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 POLINL3   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 ISRM-3    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
 ASL-3     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
```

```
TRANSU   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSM   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKU3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKM3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKL3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCU3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCM3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCL3   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CUM-4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CMM-4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CLM-4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINU4  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINM4  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINL4  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ISRM-4   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ASL-4    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSU   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSM   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKU4   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKM4   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKL4   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCU4   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCM4   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCL4   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CUM-5    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CMM-5    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CLM-5    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINU5  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINM5  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINL5  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ISRM-5   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ASL-5    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSU   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSM   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKU5   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKM5   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKL5   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCU5   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCM5   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCL5   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CUM-6    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CMM-6    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CLM-6    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINU6  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINM6  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINL6  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ISRM-6   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ASL-6    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSU   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSM   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
```

```
TRANSL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKU6   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKM6   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKL6   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCU6   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCM6   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCL6   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CUM-7    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CMM-7    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CLM-7    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINU7  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINM7  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINL7  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ISRM-7   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ASL-7    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSU   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSM   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKU7   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKM7   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKL7   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCU7   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCM7   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCL7   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CUM-8    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CMM-8    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CLM-8    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINU8  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINM8  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINL8  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ISRM-8   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ASL-8    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSU   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSM   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKU8   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKM8   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKL8   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCU8   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCM8   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
LIGCL8   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CUM-9    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CMM-9    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
CLM-9    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINU9  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINM9  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
POLINL9  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ISRM-9   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
ASL-9    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSU   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSM   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
TRANSL   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
SINKU9   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
```